

A simple expression for the terms in the Baker-Campbell-Hausdorff series

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Abstract

A simple expression is derived for the terms in the Baker-Campbell-Hausdorff series. One formulation of the result involves a finite number of operations with matrices of rational numbers. Generalizations are discussed.

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of which may be written as a rational number times $\sigma_1^{\mu_1} \sigma_2^{\mu_2} \cdots \sigma_n^{\mu_n}$, where the μ_i are either 0 or 1 (no exponents greater than 1 occur, as explained later in this paper). Next, $\sigma_i^{\mu_i}$ is replaced with x if $\mu_i = 0$ and y if $\mu_i = 1$. Thus each σ_i that occurs (to the first power) in a term indicates that a y is to be placed at the i -th location in the product of x and y variables. For example, in the case $n = 6$, we have $T(\sigma_2 \sigma_4 \sigma_5) = xyxyyx$. The operator T is a vector-space isomorphism from the space of polynomials in the σ -variables (with $\mu_i \leq 1$) to the space of linear combinations of products that have n factors that are either x or y .

The log operation in Eq. (2.9) is simple because FG is equal to the $(n + 1) \times (n + 1)$ identity matrix (which we denote by I) plus a matrix that is strictly upper triangular. Thus the series for $\log[I + (FG - I)]$ terminates after finitely many terms.

$$\log FG = - \sum_{q=1}^n \frac{(-1)^q}{q} (FG - I)^q. \quad (2.10)$$

The calculation of z_n , the order n term in the Baker-Campbell-Hausdorff series, can therefore be carried out with a finite number of simple operations. There are no sums over partitions, operations with noncommuting variables, translations of binary sequences into descriptions in terms of block lengths, etc.

III. EXAMPLES

Let us begin by working out the example of $n = 1$. We have

$$F = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \quad (3.1)$$

and

$$G = \begin{pmatrix} 1 & \sigma_1 \\ 0 & 1 \end{pmatrix}. \quad (3.2)$$

From this follows

$$FG = \begin{pmatrix} 1 & 1 + \sigma_1 \\ 0 & 1 \end{pmatrix} \quad (3.3)$$

and

$$z_1 = T(\log FG)_{1,1+1} = T(\sigma_1^0 + \sigma_1^1) \quad (3.4)$$

$$= x + y. \quad (3.5)$$

Next let us work out the example of $n = 2$. We have

$$F = \begin{pmatrix} 1 & 1 & \frac{1}{2} \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{pmatrix} \quad (3.6)$$

and

$$G = \begin{pmatrix} 1 & \sigma_1 & \frac{1}{2}\sigma_1\sigma_2 \\ 0 & 1 & \sigma_2 \\ 0 & 0 & 1 \end{pmatrix}. \quad (3.7)$$

From this follows

$$FG = \begin{pmatrix} 1 & 1 + \sigma_1 & \frac{1}{2} + \sigma_2 + \frac{\sigma_1\sigma_2}{2} \\ 0 & 1 & 1 + \sigma_2 \\ 0 & 0 & 1 \end{pmatrix} \quad (3.8)$$

and

$$(FG - I)^2 = \begin{pmatrix} 0 & 0 & 1 + \sigma_1 + \sigma_2 + \sigma_1\sigma_2 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad (3.9)$$

so that

$$z_2 = T(\log FG)_{1,2+1} = T\left(\frac{1}{2}\sigma_1^0\sigma_2^1 - \frac{1}{2}\sigma_1^1\sigma_2^0\right) \quad (3.10)$$

$$= \frac{1}{2}(xy - yx). \quad (3.11)$$

For the case $n = 3$, the equations result in

$$z_3 = T\left(\frac{1}{12}\sigma_1 - \frac{1}{6}\sigma_2 + \frac{1}{12}\sigma_3 + \frac{1}{12}\sigma_1\sigma_2 - \frac{1}{6}\sigma_1\sigma_3 + \frac{1}{12}\sigma_2\sigma_3\right) \quad (3.12)$$

$$= \frac{1}{12}yxx - \frac{1}{6}xyx + \frac{1}{12}xxy + \frac{1}{12}yyx - \frac{1}{6}yxy + \frac{1}{12}xyy. \quad (3.13)$$

The case $n = 4$ works out to be

$$z_4 = T\left(-\frac{1}{24}\sigma_1\sigma_2 + \frac{1}{12}\sigma_1\sigma_3 - \frac{1}{12}\sigma_2\sigma_4 + \frac{1}{24}\sigma_3\sigma_4\right) \quad (3.14)$$

$$= -\frac{1}{24}yyxx + \frac{1}{12}yxyx - \frac{1}{12}xyxy + \frac{1}{24}xxyy. \quad (3.15)$$

These results and higher-order calculations not shown here agree with results published in the literature [3,4]. As an example of the types of coefficients that occur, when n is 7 our formula gives a coefficient of $-1/1512$ for the $yxxxyyy$ term, and this agrees with the literature result.

IV. PROOF OF THEOREM

We begin by considering the Baker-Campbell-Hausdorff series for $\log(e^M e^N)$, where the $(n+1) \times (n+1)$ matrices M and N are defined in Eqs. (2.5) and (2.6). The matrices M and N are written out explicitly on the right-hand sides of Eqs. (2.7) and (2.8). They have nonzero elements only on the first superdiagonal. Therefore, a product having m factors that are either M or N will have nonzero elements only on the m -th superdiagonal. Thus,

the upper-right element of the matrix $\log(e^M e^N)$ is equal to the upper-right element of the matrix that is the order n term in the Baker-Campbell-Hausdorff series for $\log(e^M e^N)$. We write this as

$$[\log(e^M e^N)]_{1,n+1} = \sum_W C(W) [\Pi(W)]_{1,n+1}, \quad (4.1)$$

where the sum runs over all “words” W of length n (ordered n -tuples of elements that are either the symbol M or the symbol N), $C(W)$ denotes the coefficient of W in the order n term in the Baker-Campbell-Hausdorff series, and $\Pi(W)$ denotes a product of M and N matrices as specified by the word W .

We now show that $[\Pi(W)]_{1,n+1}$ is a product of σ -variables whose indices give the positions of the N 's in the word W . We let the matrix $\Pi(W)$ act on an $(n+1)$ -component column vector that is all zeroes except the lowest element, which is a 1. After each multiplication by an M or an N matrix, the location of the nonzero element in the column vector moves up by one step. If the matrix multiplying the column vector is an N , the nonzero element in the column vector gets multiplied by a σ . The index on the σ gives the location of the N matrix in the word W , as can be seen by looking at the structure of the N matrix, shown on the right-hand side of Eq. (2.8). After all of the n matrices in the word W have acted on the column vector, the nonzero element in the vector is at the top, and this element is a product of σ -variables whose indices describe the word W in the manner explained above. The top element of the vector obtained by letting a matrix act on the initial column vector described above is the upper-right element of the matrix. Thus we have shown that $[\Pi(W)]_{1,n+1}$ is a product of σ -variables whose indices give the positions of the N 's in the word W . This fact together with the relations $F = \exp M$ and $G = \exp N$ and Eq. (4.1) proves Eq. (2.9).

V. ALTERNATIVE FORMULATION

In this section we present a result equivalent to the result presented above, but the matrix operations involve only numbers. We will express the n -th order term, z_n , as a linear combination of terms of the form $(x + \sigma_1 y)(x + \sigma_2 y) \cdots (x + \sigma_n y)$, where the σ 's are either $+1$ or -1 . There are 2^n such terms. Our result is that the coefficient of a given term is 2^{-n} times the value of the polynomial $(\log FG)_{1,n+1}$ defined Sec. II, with the corresponding σ -values substituted in. This number can be computed by substituting the σ -values into the G matrix before doing the matrix operations. These statements can be summarized as

$$z_n = 2^{-n} \sum_{\sigma_1, \dots, \sigma_n} (\log FG)_{1,n+1} (x + \sigma_1 y)(x + \sigma_2 y) \cdots (x + \sigma_n y), \quad (5.1)$$

where the sum is over all 2^n possible assignments of ± 1 to the σ -variables.

Let us work out an example. For $n = 2$ the equation becomes

$$z_2 = 2^{-2} \sum_{\sigma_1, \sigma_2} \left(\frac{\sigma_2}{2} - \frac{\sigma_1}{2} \right) (x + \sigma_1 y)(x + \sigma_2 y) \quad (5.2)$$

$$= \frac{1}{4} \left[\left(\frac{1}{2} - \frac{-1}{2} \right) (x - y)(x + y) + \left(\frac{-1}{2} - \frac{1}{2} \right) (x + y)(x - y) \right] \quad (5.3)$$

$$= \frac{1}{2} (xy - yx), \quad (5.4)$$

where we have used Eq. (3.10).

A calculation of z_n without the use of multiplication of matrices of polynomials would proceed in the following way. For every choice of $+1$ or -1 values for the σ -variables one computes the value of $2^{-n} (\log FG)_{1,n+1}$. This involves a finite number of operations with numbers. The result is the coefficient of $(x + \sigma_1 y)(x + \sigma_2 y) \cdots (x + \sigma_n y)$ in the expression for z_n in Eq. (5.1). Next, we imagine the process of expanding all of the products $(x + \sigma_1 y)(x + \sigma_2 y) \cdots (x + \sigma_n y)$. The result of this operation is a sum over words in the variables x and y . To get the coefficient of a particular word one sums all of the coefficients calculated from $2^{-n} (\log FG)_{1,n+1}$ with a sign given by the product of the σ 's at the locations of the y 's in the word. For example, if the word is $xyyxy$ then the coefficients are summed with signs given by $\sigma_3 \sigma_4 \sigma_6$.

We now prove Eq. (5.1). We consider the order n term in $\log(e^{x+y} e^{x-y})$. This may be written in two ways,

$$\sum_{\sigma_1, \dots, \sigma_n} C(\sigma_1, \dots, \sigma_n) (x + \sigma_1 y) \cdots (x + \sigma_n y) = \sum_W C'(W) W. \quad (5.5)$$

The sum on the left-hand side is a sum over all assignments of $+1$ or -1 to the variables $\sigma_1, \dots, \sigma_n$. The coefficient $C(\sigma_1, \dots, \sigma_n)$ is the usual coefficient in the Baker-Campbell-Hausdorff series, with the σ 's identifying a word. The right-hand side of Eq. (5.5) results from multiplying out all of the products $(x + \sigma_1 y) \cdots (x + \sigma_n y)$. It is a sum over words in x and y , and $C'(W)$ denotes the resulting coefficient of the word W . [In this context we use the term "word" to denote an actual product of a certain sequence of x and y variables, because such a product does not evaluate to become something else, as it did in the case of the products of M and N matrices in the previous section. Thus, the notation $\Pi(W)$ is not needed in Eq. (5.5).] The coefficient $C'(W)$ of a particular word W can be expressed in terms of the $C(\sigma_1, \dots, \sigma_n)$. For every set of values for $\sigma_1, \dots, \sigma_n$ in the sum on the left-hand side we get a contribution to $C'(W)$ of $C(\sigma_1, \dots, \sigma_n)$ times the product of the σ 's that correspond to the y 's in W . This product is the same as the product of $\sigma_i^{(W)}$, where the $\sigma^{(W)}$ values describe the word W ($\sigma_i^{(W)}$ is $+1$ if the i -th factor in W is x , and $\sigma_i^{(W)}$ is -1 if the i -th factor in W is y), and the product runs over i -values corresponding to negative σ 's. Thus, $C'(W)$ is precisely the polynomial in $\sigma^{(W)}$ given in the first theorem. Now we transform from x and y to new variables according to $x + y = \tilde{x}$ and $x - y = \tilde{y}$. This implies $x = (\tilde{x} + \tilde{y})/2$ and $y = (\tilde{x} - \tilde{y})/2$, and the right-hand side of Eq. (5.5) (which equals $\log e^{\tilde{x}} e^{\tilde{y}}$) becomes the right-hand side of Eq. (5.1), after the tildes have been dropped, which is justified since only variables with tildes occur at that point. The n factors of $1/2$ are collected into the factor of 2^{-n} in Eq. (5.1).

VI. SYMMETRIES OF THE COEFFICIENTS

The calculation described in the penultimate paragraph of the preceding section involves repeated evaluation of $(\log FG)_{1,n+1}$ with values of $+1$ and -1 substituted in for the σ -variables. These numbers are the coefficients in the sum in Eq. (5.1). We begin this section by showing that half of the resulting numbers will be zero because of a basic symmetry of the Baker-Campbell-Hausdorff series. Then we show that some of the nonvanishing coefficients

can be obtained from other ones. These considerations reduce the computational work involved in calculating the coefficients in Eq. (5.1).

The relationship $e^z = e^x e^y$ implies $e^{-z} = e^{-y} e^{-x}$ and

$$z = -\log e^{-y} e^{-x}. \quad (6.1)$$

From this we see that swapping the x 's and y 's in the n -th order term z_n gives the same result as multiplying z_n by $(-1)^{n-1}$. In the present context, the σ -variables are being assigned values of $+1$ or -1 , so we may use the relationship $\sigma_i^2 = 1$. The preceding statement about the symmetry of z_n is equivalent to

$$(\log FG)_{1,n+1} \prod_{i=1}^n \sigma_i = (-1)^{n-1} (\log FG)_{1,n+1}. \quad (6.2)$$

Multiplication by $\prod_{i=1}^n \sigma_i$ effects a swapping of x and y , because of the relationship $\sigma_i^2 = 1$. If the number of σ 's that are $+1$ is even then $\prod_{i=1}^n \sigma_i$ will equal $(-1)^n$ because all of the σ 's in the product may be replaced with -1 without changing the value of the product. Therefore, if the number of σ 's that are $+1$ is even, then $(\log FG)_{1,n+1}$ is zero. Elementary combinatorics shows that this condition holds for one-half of the terms in the sum in Eq. (5.1). In the case of odd n greater than 1, there is one additional term which vanishes, namely the one for which all of the σ 's are $+1$. This is because the matrices M and N are equal and therefore commute. Thus $\log FG$ is equal to $M + N$ and the upper-right element of $\log FG$ is zero. [In the case of even n , $(\log FG)_{1,n+1}$ of course also vanishes when all of the σ 's are $+1$, but this vanishing has already been counted in the discussion above.]

Thus far, we have identified coefficients in the sum in Eq. (5.1) that are zero for symmetry reasons. This author has searched up through order $n = 15$ and found all of the remaining coefficients to be nonzero.

A further symmetry of $(\log FG)_{1,n+1}$ is

$$[(\log FG)_{1,n+1}](\sigma_1, \dots, \sigma_n) = (-1)^{n-1} [(\log FG)_{1,n+1}](\sigma_n, \dots, \sigma_1). \quad (6.3)$$

The notation on the left-hand side of this equation indicates explicitly that $(\log FG)_{1,n+1}$ is a function of the n variables $\sigma_1, \dots, \sigma_n$. On the right-hand side, these n quantities are inserted into the function in the reversed order. The fact that these two values of the function are related by a factor of $(-1)^{n-1}$ is due to a symmetry of the Baker-Campbell-Hausdorff series. It follows immediately from results in Ref. [1] that the coefficient of a word in the variables x and y is equal to $(-1)^{n-1}$ times the coefficient of the word obtained by reversing the order of the factors in the original word. This implies that $T\{[(\log FG)_{1,n+1}](\sigma_n, \dots, \sigma_1)\}$ (where T is the operator defined in Sec. II), which is the order n term in the Baker-Campbell-Hausdorff series with the sequence of the factors in each term reversed, is equal to $(-1)^{n-1}$ times $T\{[(\log FG)_{1,n+1}](\sigma_1, \dots, \sigma_n)\}$. Because the vector-space isomorphism T is invertible, this proves Eq. (6.3). This equation is useful because it can be used to avoid carrying out unnecessary evaluations of $(\log FG)_{1,n+1}$.

VII. COMPUTER IMPLEMENTATION

The methods presented in this paper can easily be used with computers. A simple example of how the results of Sec. II can be implemented using Mathematica is shown

below. It is not necessary to load any special packages to run this code. This example is oriented toward ease of coding. Faster implementations are possible. The first program gives the polynomial to the right of the T operator in Eq. (2.9), and the second program (for $n > 1$) translates this into z_n , the corresponding expression in terms of x and y .

```
p[n_] := p[n] = ( F = Table[1/(j-i)!,{i,n+1},{j,n+1}];
  G = Table[1/(j-i)! Product[s[k],{k,i,j-1}],{i,n+1},{j,n+1}];
  qthpower = IdentityMatrix[n+1]; FGm1 = F.G - qthpower; Expand[
  -Sum[qthpower=qthpower.FGm1; (-1)^q / q qthpower,{q,n}][[1,n+1]])

translated[n_] := (temp = Expand[Product[s[k]^2, {k,n}] p[n]];
  Sum[term = Apply[List, temp[[i]]]; term[[1]] Apply[StringJoin,
  Take[term,-n] /. {s[i_]^2->"x",s[i_]^3->"y"}], {i,Length[temp]})
```

```
In[3]:= translated[4]
```

```
Out[3]= 
$$\frac{xyxy}{24} - \frac{xyxy}{12} + \frac{yxyx}{12} - \frac{yyxx}{24}$$

```

VIII. OTHER SERIES

As in the case of Goldberg's results [1], the methods of this paper can be used to calculate $\log f(x)f(y)$, where $f(x)$ is an arbitrary power series with $f(0) = 1$. The only changes that are necessary are that occurrences of the exponential function such as those in Eqs. (2.7) and (2.8) must be replaced with the function f . The matrices M and N have the property that when they are raised to the power $n + 1$ the result is zero, so the calculation of $f(M)$ and $f(N)$ terminates after finitely many matrix operations.

IX. GENERALIZED BAKER-CAMPBELL-HAUSDORFF SERIES

The methods presented in Sec. II may also be used to calculate the terms in generalized Baker-Campbell-Hausdorff series. For example, if $z = \log e^x e^y e^w$ then the n -th order term may be found as follows. Matrices F and G are defined as in Eqs. (2.1) and (2.2), and a matrix H is defined by

$$H_{ij} = \frac{1}{(j-i)!} \prod_{k=i}^{j-1} \tau_k, \quad i, j = 1, \dots, n+1, \quad (9.1)$$

where τ_1, \dots, τ_n are n additional commuting variables. The definition of H is the same as the definition of G , except that different variables are used. Reasoning similar to that in the original case gives the following expression for z_n .

$$z_n = T(\log FGH)_{1,n+1}, \quad (9.2)$$

where the definition of the T operator now has been extended to also putting a w at the i -th position of a product of x 's, y 's and w 's for an occurrence of τ_i . For example, when n is 4, we have $T(\sigma_2 \tau_3) = xywx$. The results obtained from Eq. (9.2) agree with those obtained from Reutenauer's generalization [8] of Goldberg's theorem.

An example of how these methods can be used with Mathematica is shown below. For ease of coding, the notation has been changed slightly.

```
p3[n_] := p3[n] = (
  F = Table[1/(j-i)! Product[s[k,"x"],{k,i,j-1}],{i,n+1},{j,n+1}];
  G = Table[1/(j-i)! Product[s[k,"y"],{k,i,j-1}],{i,n+1},{j,n+1}];
  H = Table[1/(j-i)! Product[s[k,"w"],{k,i,j-1}],{i,n+1},{j,n+1}];
  qthpower = IdentityMatrix[n+1]; FGm1 = F.G.H - qthpower; Expand[
  -Sum[qthpower=qthpower.FGm1; (-1)^q / q qthpower,{q,n}][[1,n+1]]])

translated3[n_] := (temp = p3[n]; Sum[term = Apply[List, temp[[i]]]; term[[1]]*
  Apply[StringJoin, Take[term,-n] /. s[j_,k_]->k], {i,Length[temp]}])
```

```
In[3]:= translated3[2]
```

```
Out[3]= 
$$\begin{matrix} -wx & wy & xw & xy & yw & yx \\ \hline \frac{-wx}{2} & -\frac{wy}{2} & +\frac{xw}{2} & +\frac{xy}{2} & +\frac{yw}{2} & -\frac{yx}{2} \end{matrix}$$

```

X. CONCLUSION

The results contained in this paper provide a means of computing the entire n -th order term in the Baker-Campbell-Hausdorff series, without the use of noncommuting variables, sums over partitions, or other complicated operations. One application is in writing simple programs in standard computer languages to calculate the Baker-Campbell-Hausdorff series. Such programs do not result in a significant reduction in computer time needed. Rather, the programming involved is simplified. The sample program included in this paper can be shortened to just a few lines, and it is not necessary to load special software packages. The calculation of higher-order terms in the Baker-Campbell-Hausdorff series is usually done in computer languages that do not have symbol manipulation, because they are faster. This paper also explains how a simple program can be written in such a language to calculate the series.

This paper does not address the question of expressing the Baker-Campbell-Hausdorff series in terms of commutators. As explained in Sec. II, if an expression in terms of commutators is desired, the substitution due to Dynkin [3,5-7] may be used to transform the results calculated here.

Future research could include finding alternative ways to calculate certain sequences of elements in graded free Lie algebras, such as those in Ref. [13] (which also contains an interesting method of computing the Baker-Campbell-Hausdorff series by numerically integrating a differential equation). These quantities occur in the optimization of numerical

algorithms involving computations in Lie algebras. Graded Lie algebra bases can be used in the construction of Runge-Kutta methods on manifolds.

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