A note on the Zassenhaus product formula

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We provide a simple method for the calculation of the terms $c_n$ in the Zassenhaus product $e^{a+b} = e^a \cdot e^b \cdot \prod_{n=2}^{\infty} e^{c_n}$ for non-commuting $a$ and $b$. This method has been implemented in a computer program. Furthermore, we formulate a conjecture on how to translate these results into nested commutators. This conjecture was checked up to order $n = 17$ using a computer.

I. INTRODUCTION

The product of the exponentials of two non-commuting variables $x$ and $y$ may be expressed in terms of the Baker-Campbell-Hausdorff (BCH) series

$$e^x e^y = e^{x+y + \sum_{n=2}^{\infty} z_n}.$$  (1)

The terms $z_n$ of the sum may be written as linear combinations of words $W$ of length $n$ consisting of letters $x$ and $y$,

$$z_n = \sum_{W(s_1, \ldots, s_n)} z(W) W(s_1, \ldots, s_n),$$  (2)

where each word $W(s_1, \ldots, s_n)$ is a product of $n$ factors $s_i = x$ or $s_i = y$. The sum in Eq. (2) is over all possible different words, i.e. the sum over $W$ has in principle $2^n$ terms. Some of these terms vanish, because the corresponding coefficient $z(W)$ equals zero. The coefficients $z(W)$ may be determined in various ways. A simple method to determine these coefficients has been suggested recently by Reinsch [1]. His method is easily implemented in a computer program [1, 2]. Another method was presented by Goldberg [3], and his method was implemented in a program by Newman and Thompson [4].

The terms $z_n$ of the BCH series may be expressed as linear combinations of nested commutators of $x$ and $y$. This was originally shown by Baker, Campbell, and Hausdorff [5]. However, explicit determination of the coefficients was difficult for general $n$. Dynkin [6, 7] showed that the $z_n$ can be represented as

$$z_n = \frac{1}{n} \sum_{W(s_1, \ldots, s_n)} z(W) [],\ldots, [], s_1, s_2, \ldots, s_n]$$  (3)

where $[[\ldots [[s_1, s_2], s_3], \ldots], s_n]$ is a direct translation of the word $W$ into a left normal nested commutator, i.e. the order of the letters in the commutator and the word are the same. The representation of the $z_n$ in terms of commutators is not unique due to the Jacobi identity $[[x, y], z] + [[y, z], x] + [[z, x], y] = 0$ and similar identities for higher order commutators. Some of them are discussed by Oto [5]. Oto also formulates a conjecture concerning another translation of the BCH terms into a linear combination of commutators. This translation consists of fewer terms than Dynkin’s translation, but a general proof of its validity is not known to us. We have checked the validity of Oto’s conjecture up to order $n = 17$ on a computer.

It was first shown by Zassenhaus [3] that there exists a formula analogous to the BCH formula for the exponential of the sum of two non-commuting variables $a$ and $b$,

$$e^{a+b} = e^a \cdot e^b \cdot \prod_{n=2}^{\infty} e^{c_n},$$  (4)

which is known as the Zassenhaus product formula. The individual terms $c_n$ will be called the Zassenhaus exponents in the following. They may also be written in terms of words of length $n$ consisting of the letters $a$ and $b$, i.e.

$$c_n = \sum_{W(t_1, \ldots, t_n)} c(W) W(t_1, \ldots, t_n)$$  (5)
with \( t_i = a \) or \( t_i = b \). It is the goal of this note to provide a simple method for the calculation of the coefficients \( c(W) \) as well as to propose a suitable computer implementation. Our method has been developed in analogy to the procedure proposed by Reinsch [1] for the BCH terms.

The Zassenhaus exponents may also be obtained in terms of nested commutators as shown e.g., in Refs. [3][10]. Dynkin’s theorem [4] provides a (generally valid) translation of words into nested commutators, if such a translation exists. Therefore, it is possible to directly translate the expressions for the Zassenhaus exponents [5] into a linear combination of left normal nested commutators as in Eq. (3). In analogy to the conjecture by Oteo [8] for the BCH terms, we formulate here a conjecture concerning another translation of words into left normal nested commutators for the Zassenhaus exponents involving fewer terms than Dynkin’s translation. Using a computer, we found this conjecture to be valid for the Zassenhaus exponents up to order \( n = 17 \), but at this time we cannot provide a general proof.

II. THE ZASSENHAUS EXPONENTS

In this section we state a corollary which allows a recursive determination of the Zassenhaus exponents.

Let \( \tau_1, \ldots, \tau_n \) be commuting variables. In terms of these variables we define three upper triangular \((n + 1) \times (n + 1)\) matrices \( H, K, \) and \( L \) with matrix elements given by

\[
H_{ij} = \frac{1}{(j - i)!} \cdot \prod_{k=i}^{j-1} (1 + \tau_k), \quad K_{ij} = \frac{(-1)^{i+j}}{(j - i)!}, \quad L_{ij} = \frac{(-1)^{i+j}}{(j - i)!} \cdot \prod_{k=i}^{j-1} \tau_k
\]

for \( 1 \leq j \leq n \) and zero otherwise. These matrices may be expressed as exponentials of the \((n + 1) \times (n + 1)\) matrices \( P \) and \( Q \) defined by

\[
P_{ij} = \delta_{i+1,j}, \quad Q_{ij} = \delta_{i+1,j} \tau_i
\]

where \( \delta_{ij} \) is the Kronecker symbol,

\[
H = \exp(P + Q), \quad K = \exp(-P), \quad L = \exp(-Q).
\]

Furthermore, we define an operator \( U \) which operates on products \( p \) of the variables \( \tau_i \)

\[
p = \tau_1^{\mu_1} \tau_2^{\mu_2} \tau_3^{\mu_3} \ldots \tau_n^{\mu_n}
\]

with \( \mu_i \in \{0, 1\} \) for \( i = 1, \ldots, n \). The operator \( U \) “translates” such a product \( p \) into a word consisting of letters \( a \) and \( b \) according to the following rule: If \( \mu_i = 0 \), \( \tau_i^{\mu_i} \) is replaced by an \( a \), and if \( \mu_i = 1 \), \( \tau_i^{\mu_i} \) is replaced by a \( b \). The index \( i \) determines the position of the letter in the word. E.g., for \( n = 6 \) the product \( p = \tau_1^{2} \tau_2^{0} \tau_3^{1} \tau_4^{0} \tau_5^{0} = \tau_1 \tau_3 \tau_4 \) is translated as follows:

\[
U(p) = U(\tau_1^{2} \tau_2^{0} \tau_3^{1} \tau_4^{0} \tau_5^{0}) = U(\tau_1 \tau_3 \tau_4) = babaa.
\]

The operator \( U \) is a vector-space isomorphism mapping the space of polynomials in the \( \tau \)-variables (with \( \mu_i = 0 \) or \( \mu_i = 1 \)) into the space of words of length \( n \).

**Corollary 1** The Zassenhaus exponent \( c_2 \) defined in Eq. (4) is obtained in terms of the \( 3 \times 3 \) matrices \( L, K, H \) as \( c_2 = U(L \cdot K \cdot H)_{1,3} \). For \( n > 2 \), the Zassenhaus exponents \( c_n \) are given in terms of the corresponding \((n + 1) \times (n + 1)\) matrices as

\[
c_n = U \left( \left( e^{-c_{n-1}} \cdot \ldots \cdot e^{-c_2} \cdot L \cdot K \cdot H \right)_{1,n+1} \right)
\]

Here, \( C_m \), \( 1 < m < n \) are the Zassenhaus exponents written in terms of the \((n + 1) \times (n + 1)\) matrices \( P \) and \( Q \), and the index \( 1, n+1 \) indicates the upper right element of a matrix.

This corollary permits a recursive determination of the Zassenhaus exponents. In fact, due to the special structure of the matrices \( P \) and \( Q \) all exponents in Eq. (10) are obtained as finite sums, and the whole calculation can be done in a finite amount of steps either by hand or on a computer. A suitable computer implementation will be presented in section [5].
A. Examples

Before proving Corollary 1 we work out a number of examples. For \( n = 2 \) we need to use the \( 3 \times 3 \) matrices given by

\[
L = \begin{pmatrix}
1 & -\tau_1 & \frac{1}{2}\tau_1\tau_2 \\
0 & 1 & -\tau_2 \\
0 & 0 & 1
\end{pmatrix},
\quad
K = \begin{pmatrix}
1 & -1 & \frac{1}{2} \\
0 & 1 & -1 \\
0 & 0 & 1
\end{pmatrix},
\quad
H = \begin{pmatrix}
1 & (1 + \tau_1) & \frac{1}{2}(1 + \tau_1)(1 + \tau_2) \\
0 & 1 & (1 + \tau_2) \\
0 & 0 & 1
\end{pmatrix}.
\]

Then,

\[
L \cdot K \cdot H = \begin{pmatrix}
1 & 0 & \frac{1}{2}\tau_1 - \frac{1}{2}\tau_2 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{pmatrix},
\]

and the second Zassenhaus exponent takes the form

\[
c_2 = U(L \cdot K \cdot H)_{1,n+1} = U \left(\frac{1}{2} \sum_{i=1}^{n} (1 + \tau_i) \right) = \frac{1}{2}(ba - ab).
\]

For \( n = 3 \) we need to use the \( 4 \times 4 \) matrices

\[
L = \begin{pmatrix}
1 & -\tau_1 & \frac{1}{2}\tau_1\tau_2 & -\frac{1}{6}\tau_1\tau_2\tau_3 \\
0 & 1 & -\tau_2 & \frac{1}{2}\tau_2\tau_3 \\
0 & 0 & 1 & -\tau_3 \\
0 & 0 & 0 & 1
\end{pmatrix},
\quad
K = \begin{pmatrix}
1 & -1 & \frac{1}{2} & -\frac{1}{3} \\
0 & 1 & -1 & \frac{1}{3} \\
0 & 0 & 1 & -1 \\
0 & 0 & 0 & 1
\end{pmatrix},
\quad
H = \begin{pmatrix}
1 & (1 + \tau_1) & \frac{1}{2}(1 + \tau_1)(1 + \tau_2) & \frac{1}{6} \sum_{i=1}^{3} (1 + \tau_i) \\
0 & 1 & (1 + \tau_2) & \frac{1}{2} \sum_{i=2}^{3} (1 + \tau_i) \\
0 & 0 & 1 & (1 + \tau_3) \\
0 & 0 & 0 & 1
\end{pmatrix},
\]

and the matrices \( P \) and \( Q \) defined in Eq. (8)

\[
P = \begin{pmatrix}
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0
\end{pmatrix}
\quad
\text{and}
\quad
Q = \begin{pmatrix}
0 & \tau_1 & 0 & 0 \\
0 & 0 & \tau_2 & 0 \\
0 & 0 & 0 & \tau_3 \\
0 & 0 & 0 & 0
\end{pmatrix}.
\]

It follows from Eq. (11) that

\[
e^{-C_2} = \exp \left( -\frac{1}{2} (Q \cdot P - P \cdot Q) \right)
= \begin{pmatrix}
1 & 0 & \frac{1}{2}(\tau_2 - \tau_1) & 0 \\
0 & 1 & 0 & \frac{1}{2}(\tau_3 - \tau_2) \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}.
\]
Therefore, the third Zassenhaus exponent takes the form

\[ c_3 = U \left( e^{-C_2} \cdot L \cdot K \cdot H \right)_{1,n+1} \]

\[ = U \left( \frac{2}{3} \tau_1 \tau_3 - \frac{1}{3} \tau_2 \tau_3 - \frac{1}{3} \tau_1 \tau_2 + \frac{1}{6} \tau_1 + \frac{1}{6} \tau_3 \right) \]

\[ = \frac{2}{3} bab - \frac{1}{3} aba - \frac{1}{3} abb - \frac{1}{3} bba + \frac{1}{6} baa + \frac{1}{6} aab. \]

In an analogous way one obtains for \( c_4 \)

\[ c_4 = \frac{1}{24} aab - \frac{1}{8} aaba + \frac{1}{8} aabb - \frac{1}{8} abaa \]

\[ + \frac{1}{4} abab - \frac{1}{8} abbb + \frac{1}{24} baaa + \frac{1}{4} baba \]

\[ + \frac{3}{8} babb - \frac{1}{8} bbaa - \frac{3}{8} bbab + \frac{1}{8} bbb. \]

These results all agree with the standard results given in the literature, see e.g. Ref. [11].

III. PROOF OF COROLLARY 1

The \((n + 1) \times (n + 1)\) matrices \(P\) and \(Q\) have non-zero elements only in their first superdiagonal. A product of \(m\) factors \(P\) or \(Q\) is a \((n + 1) \times (n + 1)\) matrix which contains non-zero elements only in the \(m\)th superdiagonal. In particular, a product of \(n\) factors \(P\) or \(Q\) has only one non-zero element in its upper right corner. A product of \(k\) factors \(P\) or \(Q\) with \(k > n\) is a null matrix.

Each Zassenhaus exponent \(c_n\) is a linear combination of words of length \(n\). As a consequence, \(C_n\) is a \((n + 1) \times (n + 1)\) matrix, which has a non-zero entry only in its upper right corner, and for each \(n \in \mathbb{N}\)

\[ e^{P+Q} = e^P \cdot e^Q \cdot \prod_{i=1}^{n} e^{C_i}. \]  

(12)

is obtained in terms of a finite product with \(n\) factors. Therefore, one obtains

\[ e^{C_n} = e^{-C_{n-1}} \cdot \ldots \cdot e^{-C_2} \cdot e^{-Q} \cdot e^{-P} \cdot e^{P+Q}. \]  

(13)

The exponentials can be calculated from a finite sum.

Since \(C_n\) only has one non-zero element in its upper right corner, it holds that \(e^{C_n} = I + C_n\), and we find

\[ (C_n)_{1,n+1} = \left( \sum c(A_1 \ldots A_n) A_1 \ldots A_n \right)_{1,n+1} \]

\[ = (e^{C_n})_{1,n+1} \]

\[ = (e^{-C_{n-1}} \cdot \ldots \cdot e^{-C_2} \cdot e^{-Q} \cdot e^{-P} \cdot e^{P+Q})_{1,n+1}, \]  

(14)

where \(A_i = P\) or \(A_i = Q\), and the sum runs over all different matrix products \(A_1 \ldots A_n\). The next step is to show that the upper-right element of a product matrix \(A_1 \ldots A_n\) is given by a product of \(\tau_i\), and that the indices on the \(\tau_i\) variables determine the positions of the \(Q\)'s in the matrix product \(A_1 \ldots A_n\). This has been shown in Ref. [12] and is not repeated here. Applying the operator \(U\) on this product of \(\tau_i\) then transforms the result Eq. (14) into a linear combination of words in terms of the letters \(a\) and \(b\). This proves Corollary 1.

IV. COMPUTER IMPLEMENTATION

The following Mathematica program implements Corollary 1. Calling it will return the Zassenhaus exponent \(c_n\) in terms of the variables \(a\) and \(b\).

The program consists of three parts: First the matrices \(L, K, H, P\) and \(Q\) are defined. Then the product of exponentials as required by Corollary 1 is calculated (starting from \(n = 2\)), and finally the translation \(U\) is implemented. The program works with strings in order to prevent Mathematica from sorting the words alphabetically.
\[ ZH[n_,a_,b_] := Module[{C,L,K,H,P,Q,m,t,r,i,j,k,u,z}, \]
\[ C[2]=(t[1]ˆ2 t[2])/2-(t[1] t[2]ˆ2)/2; \]
\[ For[m = 2, m <= n, m++, \]
\[ L = Table[(-1)ˆ(i+j)/(j-i)! Product[t[k],{k,i,j-1}],{i,m+1},{j,m+1}]; \]
\[ K = Table[(-1)ˆ(i+j)/(j-i)! , {i,m+1},{j,m+1}]; \]
\[ H = Table[1/(j-i)! Product[(1+t[k]),{k,i,j-1}],{i,m+1},{j,m+1}]; \]
\[ P = Table[KroneckerDelta[i+1,j],{i,m+1},{j,m+1}]; \]
\[ Q = Table[KroneckerDelta[i+1,j] t[i],{i,m+1},{j,m+1}]; \]
\[ C[m] = Expand[(Dot @@ Table[MatrixExp[-Sum[r = (List @@ C[m-u][[z]]) /. {t[i_] -> P, t[i_]ˆ2 -> Q}; r[[1]] (Dot @@ Take[r,-Length[r]+1]), {z,Length[C[m-u]]})],{u,1,m-2}]).L.K.H)[[1, m+1]] Product[t[j],{j,m}]]; \]
\[ Sum[r = (List @@ C[n][[k]]) /. {t[i_] -> ToString[a], t[i_]ˆ2 -> ToString[b]; r[[1]]] (StringJoin @@ Take[r,-n]), {k, Length[C[n]]}) ]; \]

More elegant but less readable Mathematica implementations than the one given above are possible, e.g. using NestList instead of a For loop. Since the Zassenhaus exponents for larger \( n \) are rather lengthy expressions, the computer needs a significant amount of memory for this calculation. On a standard personal computer with 2 GB of memory we could obtain the Zassenhaus exponents up to \( n = 17 \) within about one hour of computer time.

V. EXPRESSION IN TERMS OF COMMUTATORS

In the introduction we briefly discussed Dynkin’s translation [6,7] of words into commutators, which is applicable, whenever such a translation exists. Since it is known that a representation in terms of commutators exists for the Zassenhaus exponents [9,10], we may directly use Dynkin’s prescription in order to obtain an explicit representation of the Zassenhaus exponents in terms of commutators. We checked the validity of this procedure using a computer up to order \( n = 17 \). A translation for the BCH terms into commutators involving fewer terms than Dynkin’s prescription was proposed by Oteo [8]. To our knowledge the validity of this translation has never been proved in general. Oteo showed it to be valid up to order \( n = 10 \), and we checked this conjecture up to order \( n = 17 \) on a computer.

In analogy to Oteo’s prescription for the BCH terms, we now write down an expression for the Zassenhaus exponents

\[ c_n = \sum_{W(t_1,..,t_n)} c(W) W(t_1,..,t_n) \] (15)

in terms of commutators. The words \( W \) consist of letters \( a \) and \( b \); \( n_a(W) \) counts the number of \( a \)'s in that word. Analogously, \( n_b(W) = n - n_a(W) \) counts the number of \( b \)'s in the word \( W \). We conjecture that the Zassenhaus exponent \( c_n \) may be expressed in terms of the left normal commutator as follows

\[ c_n = \sum_{W(t_1,..,t_n) \atop t_1 \in a, t_2 \in b} \frac{c(W) \left[[..[[t_1,t_2],t_3],[..,t_n]\right]}{n_b(W)} \] (16)

Here we only sum over words starting with the letters \( ba \). Similarly, one may write

\[ c_n = \sum_{W(t_1,..,t_n) \atop t_1 \in b, t_2 \in a} \frac{c(W) \left[[..[[t_1,t_2],t_3],[..,t_n]\right]}{n_a(W)} \] (17)

and only sum over words starting with the letters \( ab \). We checked this conjecture up to order \( n = 17 \) using Mathematica and compared results up to order \( n = 6 \) with expressions given in the literature, e.g. in Ref. [11].
A. Example

For $n = 4$ one finds the following representation of the Zassenhaus exponent in terms of words

$$c_4 = \frac{-1}{24} aab - \frac{1}{8} aba + \frac{1}{8} ab + \frac{1}{8} aab - \frac{1}{8} abaa$$

According to our conjecture this may be translated into nested commutators as

$$c_4 = \frac{-1}{24} [[[b, a], a], a] + \frac{1}{8} [[[b, a], b], a] + \frac{1}{8} [[[b, a], b], b]$$

This result agrees with results given in the literature (e.g. in Ref. [10]).

VI. CONCLUSION

We developed a method for the calculation of the Zassenhaus exponents $c_n$ in the Zassenhaus product formula $e^{a+b} = e^a \cdot e^b \cdot \prod_{n=2}^{\infty} e^{c_n}$ for non-commuting $a$ and $b$. The method is given in Corollary 1, from which we obtain the Zassenhaus exponents in terms of words. It appears that our method is simpler and faster than previous methods (see e.g. Ref. [10]). We provide a suitable computer implementation.

We would like to mention that the method presented here can be easily generalized to the Zassenhaus product formula for $q$-deformed exponentials. (The Zassenhaus formula for $q$-deformed exponentials is discussed e.g. in Ref. [11] and references therein.)

Furthermore, we formulated a conjecture on how to translate the Zassenhaus exponents given in terms of words into a form in terms of left normal nested commutators. This representation involves fewer terms than a translation based on Dynkin’s theorem [7] and has been found to be valid for Zassenhaus exponents up to order $n = 17$ using a computer. We expect a proof of our conjecture to be possible along the lines of Dynkin’s proof for his representation of the BCH formula in terms of commutators. This proof shows essentially by direct calculation that the conjectured commutator representation is equivalent to the representation in terms of words. We will address this issue in a forthcoming paper.

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