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Numerical Values of Goldberg's Coefficients in the Series for $\log(e^x e^y)$

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For Daniel Shanks on the occasion of his 70th birthday

Abstract. The coefficients of K. Goldberg in the infinite series for $\log(e^x e^y)$ for noncommuting x and y are computed as far as words of length twenty.

1. Introduction. Let x and y be noncommuting indeterminates, and define z by $e^x e^y = e^z$. Here z is an infinite linear combination of words in x and y with rational number coefficients, and is to be regarded as a formal infinite series. That such a series exists is elementary, and it may be presented in several ways. First, we may simply write

$$z = x + y + \sum_{|w| \geq 2} g_w w;$$

that is, z is $x + y$ plus a linear combination extending over all words w in x and y having length $|w|$ at least two, g_w denoting the coefficient of the word w. It is these coefficients that are to be studied in this paper. Second, and this is a much deeper fact, z may be written as $x + y$ plus an infinite linear combination of commutator words,

$$z = x + y + \sum_{|w| \geq 2} h_w [w]. \tag{1}$$

Here, if $z = z_1 z_2 \cdots z_n$, with each z_i an x or y, then

$$[z] = [\ldots[[z_1, z_2], z_3], \ldots]$$

is the left-standardized commutator word involving the same letters as z, where as usual the commutator symbol $[u, v] = uv - vu$. The coefficient h_w is a rational number which depends on w. This famous fact, usually called the Campbell-Baker-Hausdorff formula, has applications in physics, group theory, Lie theory, differential geometry, and elsewhere. A well-known theorem of Dynkin provides a formula for the coefficients h_w in the presentation of z in terms of commutators; however, Dynkin's formula is unwieldy to use. Extensive discussions of this body of material may be found in many sources, for example, [6] or [17], with related material in [1], [2], [3], [8], [9].

In an elegant, but somewhat unnoticed, paper [4] written about 1955, K. Goldberg presented very attractive recursive procedures for computing the coefficients of the various words w in the noncommutator form of z. His procedures were so efficient

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that he could hand-compute the coefficients as far as the words of length ten in less than three hours. It is historically interesting to note that John Todd and Olga Taussky Todd assigned Goldberg the task of constructing computer software to evaluate these coefficients using the computing facility SEAC then available at the National Bureau of Standards [11], [16]. And, in fact, Goldberg did compute the coefficients for $n \leqslant 6$ in the internal memory of SEAC. It would have been possible to go to $n = 10$ using the external tape memory. However, his insight was so strong that further computer work was not needed to reach length ten, and the method he developed led to his 1957 doctoral thesis at the American University, Washington, D.C., under the supervision of Olga Taussky. As a nontrivial example of a computing effort leading to a theoretical advance, we think it appropriate to use the symbol g. for the coefficients that Goldberg studied.

Goldberg did not study the commutator form of z, but in his paper [4] did express a hope that his results for the noncommutator series would be found useful in the commutator version. That this hope is realized was shown in [13], where it was proved that one may take $h_w = g_w/|w|$; that is, simply dividing a Goldberg coefficient by the length of the word to which it belongs gives a coefficient in the commutator version of z. In view of this wider applicability of Goldberg's coefficients, we believe it worthwhile to enlarge his calculation by evaluating more coefficients. In this paper we shall do precisely that, going as far as the coefficients of words of length twenty, all of which were obtained by constructing software to implement Goldberg's algorithm on a microcomputer. The program will easily evaluate further coefficients; however, the number of coefficients grows very rapidly for longer word lengths.

Apart from expressing z in $e^x e^y = e^z$ as a formal infinite series, a discovery announced by the second author at the 1980 Auburn (Alabama) matrix theory conference [12], and publicized in [14], is that another representation of z exists that at first sight shows no infinite series, namely,

$$e^x e^y = e^{sxs^{-1} + tyt^{-1}},$$

for certain s and t dependent on x and y. In fact, it is known [12] that s and t have presentations in the form

$$s = e^{\sigma}, \qquad t = e^{\tau},$$

(the concatenation of exponentials here seems striking), and moreover, σ and τ are Lie elements (just as z was). That is, bringing series back, σ and τ possess expansions as formal series in commutators with rational number coefficients. The series giving σ and τ seem worth studying, and as an initial step toward evaluating some of their coefficients the computations reported in this article were undertaken. It will be especially interesting to have Lie presentations of σ and τ when only linearly independent commutators are used. (Note that the sum (1) extends over all commutators, not just linearly independent commutators. The reduction to linearly independent commutators is most efficiently done using an algorithm of M. Hall, Jr. [5], and software to do this is presently under construction.)

The article [14] offers further insight into the series-free version of these exponential formulas. Specifically, at the Auburn conference the second author announced the conjecture that, given Hermitian matrices H and K, there will always exist

unitary matrices U and V such that

$$e^{iH}e^{iK} = e^{i(UHU^* + VKV^*)}, \tag{2}$$

where * denotes the usual Hermitian adjoint. A proof of this conjecture, based on the recently announced results of B. V. Lidskiĭ [7] on the eigenvalues of a sum of Hermitian matrices, was outlined in [15]. Even though the most natural approach to (2) should be a simple evaluation of the commutator series for σ and τ at iH and iK, the reasoning in [15] in no way involves such tactics, a fact that at present is not understood. Perhaps the numerical computations reported here, and hopefully more of them to be reported later, will lead to a better insight into the unity of perspective underlying this class of problems. Further work toward both the computational and theoretical objectives just outlined is presently under way by both authors.

In the following sections, we first explain Goldberg's algorithm, then describe our tables of numbers, next frame some natural questions (proving one theorem), and finally give the coefficients themselves in 46 pages of tables.

2. Goldberg's Algorithm. Following [4], we first define a family $G_s(t)$ of polynomials, for $s = 1, 2, \ldots,$ as follows. Set $G_1(t) = 1$, and define

$$sG_s(t) = \frac{d}{dt}t(t-1)G_{s-1}(t), \qquad s = 2, 3, \ldots.$$

Now let w be the following word in letters x and y, in which $s_1, s_2, \ldots, s_m$ are positive integers:

$$w = x^{s_1}y^{s_2}x^{s_3}y^{s_4}\cdots(x \vee y)^{s_m}, \tag{3}$$

where $x \vee y$ is to be x if m is odd and y if m is even. Denote the word (3) by $w_x(s_1, \ldots, s_m)$, or more concisely by w_x. Goldberg's remarkable theorem is that for this word w_x, its coefficient g_{w_x} is

$$g_{w_x} = \int_0^1 t^{m'}(t-1)^{m''}G_{s_1}(t)G_{s_2}(t)\cdots G_{s_m}(t)\,dt, \tag{4}$$

with $m' = [m/2]$ and $m'' = [(m-1)/2]$, where $[\cdot]$ is the greatest integer function. Furthermore, for the word $w_y(s_1, \ldots, s_m)$ starting with y (instead of x) and having the same exponents $s_1, \ldots, s_m$, Goldberg showed that $g_{w_y} = (-1)^{n-1}g_{w_x}$, where $n = s_1 + \cdots + s_m$ is the word length. He also showed that $g_{w_x} = g_{w_y}$ if m is odd.

A consequence of these results is that only the coefficients g_{w_x} need be computed. Furthermore, another result of Goldberg's is that g_{w_x} remains unchanged if the exponents $s_1, \ldots, s_m$ are permuted, so that $s_1 \leqslant s_2 \leqslant \cdots \leqslant s_m$ may be assumed. Moreover, from these relations it follows that $g_{w_x} = 0$ whenever m is odd and $s_1 + \cdots + s_m$ is even, a fact that can serve as a check on the correctness of the computations.

A further identity, not found by Goldberg but proved in [12], [13], is that the Goldberg coefficients g_w, when summed over all cyclic rearrangements w of one fixed word W, sum to zero. This fact may also be used to check the correctness of the computations.

The coefficients $g_{\cdot}$ are intimately related to the Bernoulli numbers, and those with $m = 2$ were already expressed by Goldberg in terms of Bernoulli numbers. It is not difficult to construct additional formulas expressing various of his coefficients in terms of Bernoulli numbers, providing another avenue for checking the accuracy of the computations.

3. Description of the Tables. Near the end of this paper are two printed pages of tables giving the Goldberg coefficients through length eleven and some of the length twelve coefficients. Attached to the inside cover of this issue is a microfiche supplement giving all the coefficients through length twenty.

The entries of the table are indexed by the exponents $s_1, \ldots, s_m$ defining the word w_x, arranged in weakly increasing order. A typical line consists of these exponents, followed by the rational number g_w given as the quotient of relatively prime integers with positive denominator. The various coefficients are listed in order of word length, with length 2 first, and within each length, for increasing values of m, and for given word length and m, in lexicographic order on the exponents $s_1, s_2, \ldots, s_m$. As an example, the coefficient for the word $x^1y^3x^3y^6$ appears as:

$$1\ 3\ 3\ 6\ -23/1556755200$$

4. Discussion. It is striking how numerically tiny many of the coefficients are, even though very few of those not required to be zero by virtue of Goldberg's theorems in fact turn out to be zero. A general theme appears to be that the coefficients are numerically larger, for fixed m, when $s_1, \ldots, s_m$ are reduced. The proof of the following theorem shows generally why this is so and gives a quantitative formulation relative to the simplest word $W = xyxy \cdots x \vee y$.

THEOREM. $|g_{w_x}| \leqslant 2^{-s}|g_W| = 2^{-s}\int_0^1 t^{m'}(1-t)^{m''}\,dt$, *where* $s = s_1 + s_2 + \cdots + s_m - m$.

Proof. From the recurrence formula it is easy to see that all roots of $G_s(t)$ lie in the interval $(0,1)$, are symmetrically situated relative to $\frac{1}{2}$, and that the roots of $G_{s+1}(t)$ are strictly interlaced by the roots of $G_s(t)$. Moreover, $G_s(t)$ is monic of degree $s-1$. Thus, $G_s(t)$ is a product of $[(s-1)/2]$ quadratic factors $(t-\frac{1}{2})^2 - r^2$, where $0 < r < \frac{1}{2}$, together with one linear factor $t - \frac{1}{2}$ when $s-1$ is odd. For $0 \leqslant t \leqslant 1$, the quadratic factor is bounded in size by 4^{-1}, and the linear factor by 2^{-1}. Bounding each of the factors $G_{s_1}(t), \ldots, G_{s_m}(t)$ in the integral (4) for g_{w_x}, evidently $|g_{w_x}|$ is bounded by 2^{-s} times the integral in the statement of the theorem, and this integral in turn is g_W since $G_1(t) = 1$. □

From Goldberg's integral formula (4), it should not be too difficult to deduce an asymptotic formula for the coefficient size in terms of, say, $s_1, \ldots, s_m$. Another, and probably harder question, is obtained by noting that many of the coefficients have numerator ± 1. Are the coefficients "pseudo random" with respect to the frequency of occurrence of this numerator? If not, how is this numerator combinatorially related to the exponents $s_1, \ldots, s_m$?

As a computational check, the coefficients that Goldberg proved to be zero were examined, and indeed, they turned out to be zero. As a second check, the sum of coefficients over all cyclic shifts of a fixed word was computed in some trial cases, and indeed, it too was zero, as it should be. We think this is a very sharp check on the correctness of the computations. A third check was performed using the above-mentioned formulas for certain coefficients in terms of Bernouili numbers.

Another numerical computation of the series for $\log(e^x e^y)$ was reported many years ago [10] by Richtmyer and Greenspan. Their presentation goes approximately through left-standardized commutator words of weight eight, and follows a quite different computational method. Since the Goldberg (as amended by the result from

[13]) and Richtmyer/Greenspan methods write $\log(e^x e^y)$ in terms of linearly dependent commutator words, a term-by-term comparison of our numerical coefficients with those of Richtmyer/Greenspan is not possible. However, some interesting connections appear to exist, and these may be reported later if they turn out to be sufficiently worthwhile. A point worth mentioning is that all the coefficients of Richtmyer/Greenspan have numerator ± 1; however, this holds only because these authors did not continue to words with high enough weight.

```
GOLDBERG COEFFICIENTS,
     n=2(1)11.

2       0/1
1  1        1/2
3       0/1
1  2        1/12
1  1  1        -1/6
4       0/1
1  3        0/1
2  2        1/24
1  1  2        0/1
1  1  1  1        -1/12
5       0/1
1  4        -1/720
2  3        1/180
1  1  3        1/180
1  2  2        -1/120
1  1  1  2        -1/120
1  1  1  1  1        1/30
6       0/1
1  5        0/1
2  4        -1/1440
3  3        1/360
1  1  4        0/1
1  2  3        0/1
2  2  2        0/1
1  1  1  3        1/360
1  1  2  2        -1/240
1  1  1  1  2        0/1
1  1  1  1  1  1        1/60
7       0/1
1  6        1/30240
2  5        -1/5040
3  4        1/3780
1  1  5        -1/5040
1  2  4        1/2016
1  3  3        -1/1512
2  2  3        -1/5040
1  1  1  4        1/2016
1  1  2  3        -1/5040
1  2  2  2        -1/1120
1  1  1  1  3        -1/630
1  1  1  2  2        1/840
1  1  1  1  1  2        1/840
1  1  1  1  1  1  1        -1/140
8       0/1
1  7        0/1
2  6        1/60480
3  5        -1/10080
4  4        23/120960
1  1  6        0/1
1  2  5        0/1
1  3  4        0/1
2  2  4        0/1
2  3  3        0/1
1  1  1  5        -1/10080
1  1  2  4        1/4032
1  1  3  3        -1/3024
1  2  2  3        -1/10080
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1  1  1  1  4        0/1
1  1  1  2  3        0/1
1  1  2  2  2        0/1
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9       0/1
1  8        -1/1209600
2  7        1/151200
3  6        -1/56700
4  5        1/75600
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1  4  4        -1/17280
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2  3  4        -1/60480
3  3  3        1/45360
1  1  1  6        -1/43200
1  1  2  5        1/33600
1  1  3  4        -1/60480
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1  1  1  2  4        -1/10080
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1  1  1  1  1  1  1  2        -1/5040
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1  9        0/1
2  8        -1/2419200
3  7        1/302400
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5  5        1/67200
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1  2  7        0/1
1  3  6        0/1
1  4  5        0/1
2  2  6        0/1
2  3  5        0/1
2  4  4        0/1
3  3  4        0/1
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1  2  3  4        -1/120960
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