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Some new results in non-commutative algebra in the calculation of a two-point function

C Buzano,† M Rasetti‡§ and M Vadacchino†

† Istituto di Fisica del Politecnico, Torino, Italy

‡ Center for Theoretical Studies, University of Miami, Coral Gables, Florida

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Abstract. An explicit and finite algorithm is derived, allowing the exact expansion of $z = \exp(x + \lambda y)$ for non-commuting x and y, up to second order in λ. Such an expansion is the inverse of the usual Hausdorff–Baker–Campbell formula. The matrix elements of z are computed, and as an application, the Duhamel two-point function obtained.

1. Introduction and summary

The stronger version of Bogolubov's inequality (Bogolubov 1970) proposed by Roepstorff (1977), involving the comparison between Duhamel and the ordinary thermal two-point functions, as well as the generalised approach to Trotter's formula discussed by Suzuki (1976), have revived the interest in the explicit computation of operators of the form

$$z = \exp(x + \lambda y) \tag{1.1}$$

for non-commuting x and y.

For three such operators representing dynamical variables, say H, A and B, the Duhamel two-point function is defined by

$$(A, B) = \frac{1}{Z} \frac{\partial^2}{\partial\lambda\, \partial\mu} \mathrm{Tr}(\mathrm{e}^{-\beta H + \lambda A + \mu B})|_{\lambda = \mu = 0} \tag{1.2}$$

where $Z = \mathrm{Tr}(\mathrm{e}^{-\beta H})$ is the canonical partition function for temperature $T = 1/\beta$, and H is the Hamiltonian. Obviously, within the context of an application such as that of equation (1.2), the calculations are only to be made to second order in the parameter λ of (1.1). We shall therefore give, in the present paper, the explicit determination of both z and its matrix elements in a basis in which x is diagonal, up to the second order in λ. Although the problem of computing $w = \ln(\mathrm{e}^x \mathrm{e}^{\lambda y})$ over an associative but non-commutative algebraic field is an old one (Campbell 1898, Baker 1902, 1903, 1904a, b, Hausdorff 1906, Dynkin 1947) very little attention has been devoted to obtaining an analogous expansion for z¶. The inversion however, is not trivial and the combinatorics is completely different.

§ On leave from: Istituto di Fisica del Politecnico, Torino, Italy.

¶ An incomplete form of this, known as the Zassenhaus formula, was first reported by Magnus (1954) and was also used by Suzuki (1976).

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The paper is roughly divided into three main distinct parts. First in § 2, we state the problem in the framework of the theory of free Lie algebras. Such a position leads to the establishment of a system of linear equations, whose solutions are a set of rational coefficients entering the general form of the expansion of z. The system is then solved in § 3.

Finally in § 4, explicit formulae for the matrix elements of z and the two-point function (Roepstorff 1977) are derived for the particular case in which x and y are assumed to be linear operators in a Hilbert space, with a spectrum formed of eigenvalues only.

2. The inverse Hausdorff formula

As usual the ground ring is assumed to be a $\boldsymbol{Q}$ algebra. Let $X=\{x, y; x\neq y\}$ be a two-element set, L_X the free Lie algebra over X and $\hat{L}_X=\Pi_{n=0}^{\infty}L_X^n$ be the completion of L_X.

$\hat{L}_X$ is structured as a topological group when equipped with the Hausdorff composition law and it is known (Bourbaki 1960) that any element $z\in\hat{L}_X$ can then be written as a product

$$z=\prod_{\mathscr{h}\in\mathscr{L}}\mathscr{h}_{\mathscr{L}}^{\alpha(\mathscr{h})}\tag{2.1}$$

convergent in $\hat{L}_X$, where $\mathscr{L}$ is a Hall set relative to X and $\mathscr{h}_{\mathscr{L}}$ is the basic commutator of $\hat{L}_X$ defined by $\mathscr{h}$, and $\alpha(\mathscr{h})$ is a family of rational numbers.

We can therefore disregard here the questions concerning the convergence domains of the operators in (1.1) which are obviously the same as for the Baker–Campbell–Hausdorff formula and are thoroughly discussed by Dynkin (1947).

We write in general

$$\mathrm{e}^{x+\lambda y}=\mathrm{e}^{x}\,\mathrm{e}^{\lambda y}\prod_{n=2}^{\infty}{}'\,\mathrm{e}^{Q_n(x,y;\lambda)},\tag{2.2}$$

where $Q_n(x, y; \lambda)$ is an element of the free ring with two generators, x and y, and rational coefficients (because of (2.1)). Indeed $Q_n(x, y; \lambda)$ is a uniquely determined polynomial of nth degree in x and y.

The prime in equation (2.2) recalls that the product is ordered. The existence of an expansion such as (2.2) is an obvious consequence of the Hausdorff theorem. In fact let $\hat{m}$ be the ideal generated by X: the exponential map exp: $\hat{m}\to\mathbb{1}+\hat{m}$ is a bijection and the theorem implies the existence of one and only one element in $\hat{m}$ such that its exponential equals the product of the exponentials of two elements of $\hat{m}$ (Serre 1965).

Up to second order in λ, we can set

$$Q_n(x,y;\lambda)=\lambda q_n^{(1)}(x,y)+\lambda^2q_n^{(2)}(x,y)+\mathrm{O}(\lambda^3)\tag{2.3}$$

where $q_n^{(j)}(x, y)$ again denotes a homogeneous polynomial of degree n in x and y, but of degree j in y. Since Q_n is a Lie element of the free algebra A, generated by x and y, we can also write

$$q_n^{(1)}(x,y)=\alpha^{(n)}S_{n-1}\qquad n\geqslant2\tag{2.4}$$

and

$$q_n^{(2)}(x, y)=\begin{cases}\sum_{k=1}^{n-2} \alpha_k^{(n)} S_{n-1}^{(k)} & n \geqslant 3 \\ 0 & n=2\end{cases} \tag{2.5}$$

where

$$S_N=\underbrace{[[\ldots[[x, y], \ldots x], x]}_{N\text{-brackets}} \tag{2.6}$$

and

$$S_N^{(m)}=\underbrace{\overset{1,\ldots m-1,\;\; m,\; m+1,\ldots \quad N-1}{[[[\ldots[[x, y], x], \ldots x], y], \quad x], \ldots x] \; x]}}_{N\text{-brackets}} \qquad 1 \leqslant m \leqslant N-1. \tag{2.7}$$

Notice that the degree of both S_N and $S_N^{(m)}$ (for all m) is $N+1$. In the present note we give an explicit algorithm for computing the coefficients $\alpha^{(n)}$ and $\alpha_k^{(n)}$ of equations (2.4) and (2.5). The multiple commutators S_N and $S_N^{(m)}$ are related to each other by a recursive set of commutation relations, which read respectively

$$S_{N+1}=[S_N, x]; \qquad S_1=[x, y] \tag{2.8}$$

and

$$S_{N+1}^{(m)}=\begin{cases}[S_N^{(m)}, x] & \text{for } 1 \leqslant m \leqslant N-1, N \geqslant 2 \\ [S_N, y] & \text{for } m=N, N \geqslant 2.\end{cases} \tag{2.9}$$

By simple induction equations (2.8) generate a recursion relation which can be solved explicitly:

$$S_N=-\sum_{r=0}^{N}(-1)^r\binom{N}{r} x^r y x^{N-r}. \tag{2.10}$$

Then from equations (2.9) and (2.10)†

$$S_N^{(m)}=-\sum_{r=0}^{m} \sum_{s=0}^{N-m-1}(-1)^{r+s}\binom{m}{r}\binom{N-m-1}{s}$$
$$\times[x^{r+s} y x^{m-r} y x^{N-m-s-1}+(-1)^{N-m} x^{N-m-s-1} y x^r y x^{m+s-r}]. \tag{2.11}$$

While the S_N are (for different N's) obviously independent of one another, not all the $S_N^{(m)}$ are necessary to form a basis of A in that they satisfy a set of linear identities of the form

$$-[S_\nu, S_\nu]=\sum_{i=0}^{\nu}(-1)^i\binom{\nu}{i} S_{2\nu+1}^{(\nu+i)}=0, \tag{2.12}$$

one for each integer $\nu>0$.

Identity (2.12) can be proved inductively after some algebra. It allows the determination of the lower summation limit for k in equation (2.5), such that the terms in the sum do indeed belong to a ring of independent operators in the algebra, and

† An expansion analogous to equation (2.11) has been discussed by Guenin (1968).

$q_n^{(2)}(x, y)$ is in fact a Lie element of A (Friedrichs 1953)

$$q_n^{(2)}(x,y)=\begin{cases}\sum_{k=[\frac{1}{2}n]}^{n-2}\alpha_k^{(n)}S_{n-1}^{(k)} & n\geq 3\\ 0 & n=2\end{cases} \tag{2.13}$$

where $[\xi]$ denotes the maximum integer less than or equal to ξ.

We have now all we need to tackle the main problem. This can be done by expanding both sides of equation (2.2) as formal power series and then comparing on both sides the corresponding homogeneous terms of degree n and of given order $j (j=1,2)$ in λ.

Observing that the first order in λ of

$$(x+\lambda y)^N=x^N+\lambda\sum_{r=0}^{N-1}x^ryx^{N-r-1}+\lambda^2\sum_{r=0}^{N-2}\sum_{s=0}^{N-r-2}x^ryx^syx^{N-r-s-2}+\mathrm{O}(\lambda^3) \tag{2.14}$$

is a linear combination where the S_n only enter, the above procedure leads immediately, by the use of equation (2.10) to

$$\alpha^{(n)}=-1/n!. \tag{2.15}$$

3. Determination of the coefficients $\alpha_k^{(n)}$

The calculation of the second-order coefficients $\alpha_k^{(n)}$, $[\frac{1}{2}n]\leq k\leq n-2$ is more involved.

First one must write down a recursion relation for $q_n^{(2)}(x, y)$. After some non-trivial algebraic manipulations, this is found to be

$$\begin{aligned}q_n^{(2)}(x,y)=&-\sum_{j=1}^{n-3}\frac{1}{j!}x^jq_{n-j}^{(2)}(x,y)-\sum_{j=0}^{n-3}\frac{1}{j!}x^jyq_{n-j-1}^{(1)}(x,y)\\&-\frac{1}{2}\sum_{j=0}^{n-4}\frac{1}{j!}\{1-(n-j)+2[\tfrac{1}{2}(n-j)]\}x^j(q^1_{[\frac{1}{2}(n-j)]}(x,y))^2\\&-\sum_{j=0}^{n-4}\frac{1}{j!}\sum_{l=2}^{[\frac{1}{2}(n-j-1)]}x^jq_l^{(1)}(x,y)q_{n-j-l}^{(1)}(x,y)\\&-\frac{1}{2(n-2)!}x^{n-2}y^2+\frac{1}{n!}\sum_{r=0}^{n-2}\sum_{s=0}^{n-r-2}x^ryx^syx^{n-r-s-2}.\end{aligned} \tag{3.1}$$

By inserting into (3.1) the explicit expression for $q_n^{(1)}(x, y)$ obtained from (2.4), (2.10) and (2.15), equation (3.1) itself can be rewritten in the more compact form

$$q_n^{(2)}(x,y)=-\sum_{j=1}^{n-3}\frac{1}{j!}x^jq_{n-j}^{(2)}(x,y)+\sum_{r=0}^{n-2}\sum_{s=0}^{n-r-2}A_{r,s}^{(n)}x^ryx^syx^{n-r-s-2} \tag{3.2}$$

where the $\frac{1}{2}n\,(n-1)$ coefficients $A_{r,s}^{(n)}$ $(0\leq r\leq n-2; 0\leq s\leq n-2)$ can be explicitly calculated by collecting similar homogeneous terms on the right-hand side of equation (3.1). In the further developments we will consider the $A_{r,s}^{(n)}$ as known parameters. We do not give their explicit expression here though, since—as will become apparent in the following—only a subset of them corresponding to a special choice of the range of indexes r and s will be needed in the final algorithm for the $\alpha_k^{(n)}$.

Recursion relation (3.2) can be solved in the form

$$q_n^{(2)}(x, y) = \sum_{r=0}^{n-2} \sum_{s=0}^{n-r-2} \omega_{r,s}^{(n)} x^r y x^s y x^{n-r-s-2} \tag{3.3}$$

with

$$\omega_{r,s}^{(n)} = (-1)^r \sum_{j=0}^{r} \frac{(-1)^j}{(r-j)!} A_{j,s}^{(n-r+j)}. \tag{3.4}$$

Upon substitution of (3.3) (and (3.4)) on the left-hand side of equation (2.13) and of (2.11) on the right-hand side, one obtains by comparing similar terms, the required system of equations in $\alpha_k^{(n)}$.

Notice that not all the equations one can possibly write in this way are to be used. In fact it is easily checked that only $[\frac{1}{2}(n-1)]$ are independent (which is just the number of unknowns we have), while the remaining $[\frac{1}{2}(n-1)^2+\frac{1}{2}]$ are either redundant, i.e. linear combinations of the previous ones, or they are not equations at all, in the sense that the unknowns do not appear (have coefficient zero) and they reduce to identities in the $\omega_{r,s}^{(n)}$.

One possible choice of the indexes r, s which singles out all the necessary and sufficient equations can be compactly written as

$$\boldsymbol{\Omega}_n = T_n \boldsymbol{A}_n \tag{3.5}$$

where $\boldsymbol{\Omega}_n$ and $\boldsymbol{A}_n$ are $[\frac{1}{2}(n-1)]$-component vectors of the form

$$\boldsymbol{\Omega} \equiv \begin{pmatrix} \omega_{0,0}^{(n)} \\ \omega_{1,0}^{(n)} \\ \vdots \\ \omega_{[\frac{1}{2}(n-1)],0}^{(n)} \end{pmatrix} \qquad \boldsymbol{A}_n \equiv \begin{pmatrix} \alpha_{[\frac{1}{2}n]}^{(n)} \\ \alpha_{[\frac{1}{2}n]+1}^{(n)} \\ \vdots \\ \alpha_{n-2}^{(n)} \end{pmatrix} \tag{3.6}$$

respectively, and T_n is a $[\frac{1}{2}(n-1)] \times [\frac{1}{2}(n-1)]$ matrix whose non-zero elements are given by

$$(T_n)_{ij} = (-1)^{i+1} \binom{[\frac{1}{2}(n-1)]-j}{i-1} \qquad \text{for } 1 \leqslant i \leqslant [\tfrac{1}{2}(n+1)]-j; \qquad 1 \leqslant j \leqslant [\tfrac{1}{2}(n-1)]. \tag{3.7}$$

In other words T_n is triangular and non-singular. The simple inversion of equation (3.5) then gives

$$\alpha_{[\frac{1}{2}(n-2)]+i}^{(n)} = (-1)^{[\frac{1}{2}(n-1)]+i} \sum_{t=[\frac{1}{2}(n+1)]-i}^{[\frac{1}{2}(n-1)]} \binom{t-1}{[\frac{1}{2}(n-1)]-i} \omega_{t-1,0}^{(n)}; \qquad 1 \leqslant i \leqslant [\tfrac{1}{2}(n-1)]. \tag{3.8}$$

Now, for the relevant subset of indexes $s=0$, $0 \leqslant j \leqslant [\frac{1}{2}(n-3)]$

$$A_{j,0}^{(n)} = \frac{1}{n!}\left(1 - \binom{n}{j+1}\right) \tag{3.9}$$

and, inserting into (3.4) and (3.8), we can finally write (3.8) in the form

$$\alpha_k^{(n)} = (-1)^{n+k} \frac{1}{n!} \sum_{s=n-k-1}^{[\frac{1}{2}(n-1)]} (-1)^s \binom{n-1}{s} \binom{s-1}{n-k-2}; \qquad [\tfrac{1}{2}n] \leqslant k \leqslant n-2. \tag{3.10}$$

Equation (3.10) is the algorithm for explicit computation of $q_n^{(2)}(x, y)$, by (2.13), for any n. For the sake of convenience we list in table 1 the numerical values of $\beta_k^{(n)} = n!\alpha_k^{(n)}$ for $3 \leqslant n \leqslant 12$, for all k (of course $n = 2$ is not included because no multiple commutator of degree two including two y's exists).

Table 1. $\beta_k^{(n)} = n!\alpha_k^{(n)}$

$n \backslash k$	1	2	3	4	5	6	7	8	9	10
3	−2									
4		−3								
5		−6	2							
6			−10	5						
7			−20	25	−11					
8				−35	49	−21				
9				−70	154	−126	34			
10					−126	294	−246	69		
11					−252	798	−1002	573	−127	
12						−462	1518	−1947	1133	−253

4. Matrix elements and the two-point function

In most of the physical applications, x is a linear self adjoint operator in a Hilbert space, whose spectrum is formed by eigenvalues only. Hereafter we compute the matrix elements of z up to second order in λ under this hypothesis. Even though the case when x is a generic self adjoint operator should require only minor formal variations, it will not be treated here.

In order to do so, we choose a complete, orthonormal basis $\{|j, m\rangle\} \in \mathscr{H}$ where $\mathscr{H}$ is the Hilbert space in which x and y are acting, namely

$$x|jm\rangle = x_j|jm\rangle; \qquad (\langle jm|j'm'\rangle = \delta_{jj'}\delta_{mm}; \sum_{jm}|jm\rangle\langle jm| = 1). \tag{4.1}$$

m labels the n_j vectors in $\mathscr{H}$ corresponding to the same eigenvalue x_j.

Then we define three auxiliary functions

$$F(\xi) = \sum_{N=0}^{\infty} \frac{1}{(N!)^2}\xi^N \tag{4.2}$$

$$G(\xi, \eta) = \sum_{N=1}^{\infty} \frac{\mathscr{G}_N(\eta)}{N!}\xi^N \tag{4.3}$$

$$E(\xi, \eta) = \sum_{N=0}^{\infty} \frac{e_N(\eta)}{N!}\xi^N \tag{4.4}$$

where $\mathscr{G}_N(\eta)$ and $e_N(\eta)$ are Nth degree polynomials defined by

$$\mathscr{G}_N(\eta) = \sum_{k=[\frac{1}{2}N]+1}^{N} g_k^{(N)}\eta^k; \qquad g_k^{(N)} = \frac{\beta_k^{(N+2)}}{(N+1)(N+2)} \tag{4.5}$$

and

$$e_N(\eta)=\sum_{k=0}^{N}\frac{1}{k!}\eta^k \tag{4.6}$$

respectively. Notice that $\mathscr{G}_N(1)=-(2+N)^{-1}$, and $e_N(\eta)$ is connected with the incomplete gamma function (Abramowitz and Stegun 1965).

Finally we can compute $\langle jm|z|j'm'\rangle$. After some algebra we find

$$\begin{aligned}\langle jm|\mathrm{e}^{x+\lambda y}|j'm'\rangle\\ &=\mathrm{e}^{x_j}\bigg(\delta_{jj'}\delta_{mm'}+\lambda\langle jm|y|j'm'\rangle\frac{\mathrm{e}^{x_{j'}-x_j}-1}{x_{j'}-x_j}\\ &\quad+\lambda^2\sum_{j''m''}\langle jm|y|j''m''\rangle\langle j''m''|y|j'm'\rangle\,.\,f(\Delta,\Delta')+\mathrm{O}(\lambda^3)\bigg)\end{aligned} \tag{4.7}$$

where

$$\begin{aligned}f(\Delta,\Delta')&=G\Big(\Delta'-\Delta,\frac{\Delta'}{\Delta'-\Delta}\Big)-G\Big(\Delta'-\Delta,\frac{\Delta}{\Delta-\Delta'}\Big)\\ &\quad+\frac{1}{\Delta\Delta'}\Big(-\frac{1}{2}-\frac{1}{2}F(-\Delta\Delta')-\mathrm{e}^{\Delta'-\Delta}+E(-\Delta,\Delta')+\mathrm{e}^{\Delta'}\Big)\end{aligned} \tag{4.8}$$

and $\Delta=x_j-x_{j''}$ and $\Delta'=x_{j'}-x_{j''}$.

As an application of (4.7) going back to equation (1.2) we have (setting $x=-\beta H$, $y=A+\mu B/\lambda$)

$$Z=\sum_{jm}\mathrm{e}^{x_j}=\sum_j n_j\,\mathrm{e}^{x_j} \tag{4.9}$$

and we find the expression—consistent with the known integral representation of the two-point function (Bogolubov 1970)

$$(A,B)=\frac{1}{2Z}\sum_{jm}\sum_{j''m''}(\langle jm|A|j''m''\rangle\langle j''m''|B|jm\rangle+\langle j''m''|A|jm\rangle\langle jm|B|j''m''\rangle)\frac{\mathrm{e}^{x_j}-\mathrm{e}^{x_{j''}}}{x_j-x_{j''}}. \tag{4.10}$$

Equation (4.10) was obtained from (4.7) observing that

$$f(\Delta,\Delta)=\frac{1}{\Delta^2}\Big(\tilde{\mathscr{G}}(\Delta)-\frac{3}{2}-\frac{1}{2}F(-\Delta^2)+\mathrm{e}^{\Delta}+E(-\Delta,\Delta)\Big)=\frac{\mathrm{e}^{-\Delta}+\Delta-1}{\Delta^2} \tag{4.11}$$

being

$$\tilde{\mathscr{G}}(\Delta)=2\sum_{s=1}^{\infty}\alpha_{2s-1}^{(2s+1)}\,\Delta^{2s+1}. \tag{4.12}$$

Notice that only coefficients of the form

$$\alpha_{2s-1}^{(2s+1)}=\frac{1}{(2s+1)!}\Big[(-1)^s\binom{2s-1}{s}-1\Big], \tag{4.13}$$

namely those appearing in odd positions on the main upper diagonal in table 1, enter equation (4.12); so that the compact form (4.11) for $f(\Delta,\Delta)$ can be derived. Naturally when the algebra A can be integrated into a finite group, and y is a tensor operator of such a group, the matrix elements in (4.7) and (4.10) can be written—by the Wigner–Eckart theorem—as the product of a reduced matrix element ($\langle j\|y\|j''\rangle$, $\langle j''\|y\|j'\rangle$) independent of m, m' and m'', times a Clebsch–Gordan coefficient of the group itself. The sums over m'' can then be executed, and the right-hand side of equation (4.7) does indeed contain only one sum (over j'').

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