New formulas for moments and functions of the multivariate normal distribution extending Stein’s lemma and Isserlis theorem

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Abstract

We prove a formula for the evaluation of expectations containing a scalar function of a Gaussian random vector multiplied by a product of the random vector components, each one raised at a non-negative integer power. Some powers could be of zeroth-order, and, for expectations containing only one vector component to the first power, the formula reduces to Stein’s lemma for the multivariate normal distribution. On the other hand, by setting the said function inside expectation equal to one, we easily derive Isserlis theorem and its generalizations, regarding higher order moments of a Gaussian random vector. We provide two proofs of the formula, with the first being a rigorous proof via mathematical induction. The second is a formal, constructive derivation based on treating the expectation not as an integral, but as the consecutive actions of pseudodifferential operators defined via the moment-generating function of the Gaussian random vector.

Keywords: normal distribution, Stein’s lemma, Isserlis theorem, Wick’s theorem, Hermite polynomials, pseudodifferential operator

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1. Introduction and main results

Stein’s lemma \[33\] is a well-known identity of the normal distribution, with applications in statistics, see e.g. \[4\], \[35\], \[21\]. More specifically, it constitutes the starting point for the celebrated Stein’s method on the distance between distributions, see e.g. \[8\]. For the case of a scalar random variable \(X\) that follows the univariate normal distribution \(N(\mu, \sigma^2)\), Stein’s lemma reads

\[
E[g(X)X] = \mu E[g(X)] + \sigma^2 E[g'(X)], \tag{1}
\]

where \(E[\cdot]\) is the expectation operator, and prime denotes the first derivative of function \(g\). In our recent work \[17\], we extended scalar Stein’s lemma \eqref{1} for expectations containing \(X\) at an integer power \(n\):

\[
E[g(X)X^n] = \sum_{\ell=0}^{n} \binom{n}{\ell} \mu^{n-\ell} \sigma^{2(\ell-k)} E[g^{(\ell-2k)}(X)], \quad n \in \mathbb{N}. \tag{2}
\]

In Eq. \eqref{2}, \(g^{(\ell)}\) denotes the \(\ell\)th derivative of \(g\), \(\binom{n}{\ell} = \frac{n!}{\ell!(n-\ell)!}\) is the binomial coefficient, \([\cdot]\) is the floor function, and the numbers

\[
H_{\ell,k} = \frac{\ell!}{2^k k!(\ell-2k)!}, \quad k = 0, \ldots, \lfloor \ell/2 \rfloor, \tag{3}
\]

are the \textit{signless Hermite coefficients}, i.e., the absolute values of the coefficients appearing in the Hermite polynomial of \(\ell\)th order \[1, \text{ expression 22.3.11}\]. \(H_{0,k}(x) = \sum_{j=0}^{[k/2]} (-1)^j H_{j,k-j} x^{(2j-k)}\). For applications of Hermite polynomials in Probability Theory, see \[29, \text{ Sec. 2.11.5}\] Results similar to Eq. \eqref{2} have also been derived in \[23, 24\], by using Rodrigues formula.

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For a random vector $X = [X_1, \ldots, X_N]^T$ following the $N$-variate normal distribution $N(\mu, C)$, the multivariate Stein’s lemma reads [16]
\[ E[g(X)X_i] = \mu_i E[g(X)] + \sum_{j=1}^{N} C_{ij} E[\partial_j g(X)], \quad i = 1, \ldots, N, \] (4)
where $\partial_j g(X) = \frac{\partial g(X)}{\partial X_j}$ is the first partial derivative of $g(X)$ with respect to $X_j$ component. Eq. (4) is easily proven by integration by parts, using the properties of the derivatives of the $N$-variate normal distribution, see [22, Eq.347].

Recently, a formula evaluating $E[g(X)X_i^2]$ for the case of $X$ following a multivariate elliptical distribution was derived [36]. The topic of the present work is to extend Stein’s lemma, providing a formula, in closed form, of expressing the expectation $E[g(X) \prod_{i=1}^{N} X_i^{m_i}]$, for the case of $X$ being an $N$-dimensional Gaussian random vector.

**Theorem 1.** (Extended multivariate Stein’s lemma) For $X \sim N(\mu, C)$, a smooth enough function $g : \mathbb{R}^N \rightarrow \mathbb{R}$, and under the assumption that all expectations involved exist, it holds true that
\[ E[g(X) \prod_{i=1}^{N} X_i^{m_i}] = E[g(X)X^\mu] = \sum_{\ell < \mu} \binom{n}{\ell} \mu^{\mu-\ell} \sum_{K} \prod_{\ell < \ell(K)} H_{L,K} C_{\ell(K)}^{L-K} E[\partial^{\ell(K)} g(X)]. \] (5)

Let us explain now the meaning of Eq (5). Eq. (5) is expressed using multi-index [27, p. 319] and index-matrix [26, 30] notation. Under this notation, the extended multivariate Stein’s lemma (5) resembles in form the respective result (2) for the scalar case. Multi-indices are denoted by lowercase boldface letters, $\mathbf{n} = [n_1]_{i=1}^N \in \mathbb{N}_0^N$, and index-matrices are denoted by uppercase boldface letters, $\mathbf{L} = (\ell_{ij})_{i,j=1}^N \in \mathbb{N}_0^{N \times N}$. Index-matrix $\mathbf{L}$ is, in general, non-symmetric, while index-matrix $\mathbf{K}$ is symmetric, $\mathbf{K} = \{k_{ij}\}_{i,j=1}^N \in \mathbb{N}_0^{N \times N}$, Index-matrices $\mathbf{K^{\text{max}}}(\mathbf{L}) = \{k_{ij}^{\text{max}}\}_{i,j=1}^N$, $\mathbf{L} = (\ell_{ij})_{i,j=1}^N$, $\mathbf{K} = (k_{ij})_{i,j=1}^N$ are symmetric, and are defined as:
\[ k_{ij}^{\text{max}} = \lfloor \ell_{ij}/2 \rfloor, \quad \text{and} \quad k_{ij} = \min(\ell_{ij}, \ell_{ji}) \quad \text{for} \quad i \neq j. \] (6)
\[ \tilde{\ell}_{ij} = \ell_{ij}, \quad \tilde{\ell}_{ij} = \ell_{ij} + \ell_{ji} \quad \text{for} \quad i \neq j. \] (7)
\[ \tilde{k}_{ij} = 2k_{ij}, \quad \text{and} \quad \tilde{k}_{ij} = k_{ij} \quad \text{for} \quad i \neq j. \] (8)

Partial ordering of multi-indices $\mathbf{m} \leq \mathbf{n}$ implies that $m_i \leq n_i$ for all $i = 1, \ldots, N$. Partial ordering of index-matrices $\mathbf{K} \leq \mathbf{L}$ implies that $k_{ij} \leq \ell_{ij}$ for all $i, j = 1, \ldots, N$. By $r(\mathbf{L})$ and $c(\mathbf{L})$, we denote the row-sum and column-sum vectors of index-matrix $\mathbf{L}$ respectively:
\[ r_i(\mathbf{L}) = \sum_{j=1}^{N} \ell_{ij}, \quad c_i(\mathbf{L}) = \sum_{j=1}^{N} \ell_{ji}, \quad i = 1, \ldots, N. \] (9)

By $\mathbf{C}_U$ we denote the upper triangular part of the symmetric matrix $\mathbf{C}$. Raising a vector to a multi-index power is defined as $\mathbf{m}^\mu = \prod_{i=1}^{N} m_i^{\mu_i}$. Raising an upper triangular matrix to a symmetric index-matrix power is defined as $\mathbf{C}_U^\mathbf{K} = \prod_{i=1}^{N} \prod_{j=1}^{k_{ij}} C_{ij}$. The partial derivative of $g(X)$ of multi-index order $\mathbf{m}$ is defined as $\partial^{\mathbf{m}} g(X) = \prod_{i=1}^{N} \partial^{m_i} g(X)$. Also, we introduce the multinomial coefficient $\binom{n}{\ell}$ of a multi-index vector and an index-matrix with respect to the rows of the matrix, called the $r$-multinomial coefficient henceforth:
\[ \binom{n}{\ell} = \frac{n!}{(n-r(\ell))!r!(\ell-k)!}. \] (10)

The factorial of a multi-index is defined as $n! = \prod_{i=1}^{N} n_i!$. The factorial of an index-matrix is defined as $L! = \prod_{j=1}^{N} \prod_{j=1}^{k_{ij}} \ell_{ij}!$. Last, the coefficients $H_{L,K}$ are defined as
\[ H_{L,K} = \frac{L!}{2^{r(k)} K_U!(L-K)!}. \] (11)

where $tr(\mathbf{K}) = \sum_{i=1}^{N} k_{ii}$ is the trace of index-matrix $\mathbf{K}$, and $K_U! = \prod_{i=1}^{N} \prod_{j=1}^{k_{ij}} k_{ij}!$. 2
Table 1: Matrix calculations for Example 1.

| $L$ | $[^L_{\sigma}]$ | $L_{\sigma}$ | $k^{\text{max}}$ | $k$ | $K$ | $H_{L,K}$ | $e(L-K)$ |
|-----|-----------------|--------------|-----------------|-----|-----|-----------|-----------|
| $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ | $\begin{bmatrix} 1 \\ 2 \end{bmatrix}$ | $\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$ | $\begin{bmatrix} 0 \\ 0 \end{bmatrix}$ | $\begin{bmatrix} 0 \\ 0 \end{bmatrix}$ | $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ | $\begin{bmatrix} 3 \\ 0 \end{bmatrix}$ |
| $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ | $\begin{bmatrix} 2 \\ 0 \end{bmatrix}$ | $\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$ | $\begin{bmatrix} 0 \\ 0 \end{bmatrix}$ | $\begin{bmatrix} 0 \\ 0 \end{bmatrix}$ | $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ | $\begin{bmatrix} 3 \\ 0 \end{bmatrix}$ |
| $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ | $\begin{bmatrix} 1 \\ 1 \end{bmatrix}$ | $\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$ | $\begin{bmatrix} 0 \\ 0 \end{bmatrix}$ | $\begin{bmatrix} 0 \\ 0 \end{bmatrix}$ | $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ | $\begin{bmatrix} 3 \\ 0 \end{bmatrix}$ |
| $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$ | $\begin{bmatrix} 2 \\ 0 \end{bmatrix}$ | $\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$ | $\begin{bmatrix} 0 \\ 0 \end{bmatrix}$ | $\begin{bmatrix} 0 \\ 0 \end{bmatrix}$ | $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ | $\begin{bmatrix} 3 \\ 0 \end{bmatrix}$ |
| $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$ | $\begin{bmatrix} 1 \\ 2 \end{bmatrix}$ | $\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$ | $\begin{bmatrix} 0 \\ 0 \end{bmatrix}$ | $\begin{bmatrix} 0 \\ 0 \end{bmatrix}$ | $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ | $\begin{bmatrix} 3 \\ 0 \end{bmatrix}$ |

Proof. In Sec. 2, we prove Eq. (5) rigorously, by multidimensional mathematical induction on $n \in \mathbb{N}_0$. In addition to this proof, and in order to provide the reader with more insight, we present, in Sec. 3, a constructive formal proof of theorem 1. This constructive proof is based on treating the mean value operator not as an integral, but as the sequential action of a number of pseudodifferential operators that are introduced in definition 1 via the moment-generating function of the Gaussian random vector. The action of these pseudodifferential operators is determined by their Taylor series expansions, under the formal assumption that all infinite series involved are summable.

In the following example, we illustrate the use of Eq. (5).

Example 1. For $N = 2$, $n = (1, 2)$, $\mu = 0$, and with $\sigma_1^2 := C_{11}$, $\sigma_2^2 := C_{22}$, Eq. (5) results in

$$E\left[g(X_1, X_2)X_1X_2^2\right] = (\sigma_1^2 \sigma_2^2 + 2C_{12}) E\left[\frac{\partial g(X_1, X_2)}{\partial X_1}\right] + 2\sigma_2^2 C_{12} E\left[\frac{\partial g(X_1, X_2)}{\partial X_2}\right] +$$

$$+ (2\sigma_1^2 \sigma_2^2 C_{12} + C_{12}) E\left[\frac{\partial^2 g(X_1, X_2)}{\partial X_1^2}\right] + (\sigma_1^2 \sigma_2^2 + 2\sigma_2^2 C_{12}) E\left[\frac{\partial^2 g(X_1, X_2)}{\partial X_1 \partial X_2}\right] +$$

$$+ \sigma_1^2 \sigma_2^2 C_{12} E\left[\frac{\partial^2 g(X_1, X_2)}{\partial X_1^2}\right] + \sigma_1^2 \sigma_2^2 C_{12} E\left[\frac{\partial^2 g(X_1, X_2)}{\partial X_2^2}\right].$$  \hspace{1cm} (12)

Proof. Since $\mu = 0$, the outer sum in the right-hand side of Eq. (5) extends over all index-matrices $L \in \mathbb{N}_0^{N \times N}$ with $r(L) = n = (1, 2)$. These matrices are $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$, $\begin{bmatrix} 0 \\ 2 \end{bmatrix}$, $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$, $\begin{bmatrix} 1 \\ 1 \end{bmatrix}$, $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$, $\begin{bmatrix} 0 \\ 2 \end{bmatrix}$, and $\begin{bmatrix} 1 \\ 1 \end{bmatrix}$. For each of these index-matrices, we calculate, in Table 1, the rest of the quantities appearing in each term of the $L$-sum in the right-hand side of Eq. (5). By substituting the quantities from Table 1 into Eq. (5), and after some regrouping of terms, we obtain Eq. (12). Note that Eq. (12) can also be validated by repetitive applications of Stein’s lemma, Eq. (4), for $E\left[g(X_1, X_2)X_1X_2^2\right]$.  \hspace{1cm} □
Corollary 1 (Product moment formula for Gaussian vectors). For the random vector \( X \sim N(\mu, C) \), the following formula for its product moments holds true:

\[
E_0[X^n] = \sum_{\mathcal{K}\in\mathcal{N}_{\text{sym}}} d_{n,K} \mu^{n-r(\mathcal{K})} C_{U}^{\mathcal{K}},
\]

where \( \mathcal{K} \) is defined from \( K \) using Eq. (8), and

\[
d_{n,K} = \frac{n!}{2^{r(\mathcal{K})} K_U! [n-r(\mathcal{K})]!}.
\]

Summation in the right-hand side of Eq. (13) extends over all index-matrices \( \mathcal{K} \) for which the respective index-matrix \( \mathcal{K} \) satisfies the condition \( r(\mathcal{K}) \leq n \).

Proof. Eq. (13) has been proven by Song and Lee in [31], using Price’s theorem, see [25, Sec. 5.3.2]; see also the recent work [11]. Here, we easily derive Eq. (13) by setting \( g(X) = 1 \) in formula (5). By setting \( g(X) = 1 \), all derivatives in the right-hand side of Eq. (5) are zero, except for the zeroth order derivative, that is for \( c(L - \hat{K}) = 0 \). By the definition relation (8) of \( \hat{K} \), \( c(L - \hat{K}) = 0 \) is achieved for \( L = \hat{K} \). Last, coefficients \( d_{n,K} \) are calculated as

\[
\binom{n}{\mathcal{K}} H_{\mathcal{K},K} = \frac{n!}{[n-r(\mathcal{K})]! K_U! 2^{r(\mathcal{K})} K_U!} = d_{n,K}.
\]

Substitution of the above in Eq. (5) results in Eq. (13).

Corollary 2 (Isserlis theorem). From Eq. (13), we derive the formula for the higher order moments of an \( N \)-dimensional Gaussian random vector \( X \) with zero mean value:

\[
E_0 \left[ \prod_{i=1}^{N} X_i \right] = \begin{cases} 
0 & \text{for } N \text{ odd,} \\
\sum_{\mathcal{P}\in\mathcal{\mathcal{P}}_N} \prod_{(i,j)\in\mathcal{P}} C_{ij} & \text{for } N \text{ even,}
\end{cases}
\]

with \( \mathcal{P}_N \) being the set of all partitions of \( \{1, \ldots, N\} \) into unordered pairs. Eq. (15) has been proven by Isserlis [13], and is also known in physics literature as Wick’s theorem [37]. For a review of the related literature see also [34].

Proof. For \( \mu = 0 \) and \( n = 1 \), the summation in Eq. (13) extends over all \( K \) with \( r(\mathcal{K}) = 1 \). Since the diagonal elements of \( \mathcal{K} \) are even numbers (see definition relation (8)), \( \mathcal{K} \) in this case has zero diagonal elements, and it is equal to \( \mathcal{K} \).

Also, we calculate that \( d_{1,K} = 1 \). Thus, Eq. (13) reads

\[
E_0 \left[ \prod_{i=1}^{N} X_i \right] = \sum_{\mathcal{K}\in\mathcal{\mathcal{A}}_N} C_{U}^{\mathcal{K}}
\]

where \( \mathcal{A}_N \) is the set of all \( N \times N \) matrices that are i) symmetric, ii) have all diagonal elements zero, iii) their elements are either 0 or 1, iv) each row sum equals to one. Thus, matrices \( \mathcal{K} \in \mathcal{\mathcal{A}}_N \) are identified [3, definition 2.1] as the adjacency matrices of undirected 1-regular graphs between \( N \) nodes. By virtue of the handshaking lemma [7, theorem 2.1], the number of nodes \( N \) cannot be of the same parity with 1, which is the graph degree. Thus, for \( N \) odd, the set \( \mathcal{A}_N \) is empty and so the odd moments are zero. For even \( N \), each undirected 1-regular graph between \( N \) nodes is equivalent to one partition of set \( \{1, \ldots, N\} \) into unordered pairs, and so Eq. (16) is expressed equivalently as the branch of Eq. (15) for even \( N \).
Base case: \( n = e^{(i)} \), \( i = 1, \ldots, N \). The index-matrices \( L \) with \( r(L) \leq e^{(i)} \) are: i) the zero matrix \( 0 \), ii) the matrices \( E^{e^{(i)}}_{E^{0}} \), \( j = 1, \ldots, N \). Matrix 0 results in the term \( \mu_0 E[g(X)] \) in the \( L \)-sum of Eq. (5). For each matrix \( E^{e^{(i)}}_{E^{0}} \), \( j = 1, \ldots, N \), we calculate that \( \left( E^{e^{(i)}}_{E^{0}} \right)_j = 1 \). \( K^{\max}(E^{e^{(i)}}_{E^{0}}) = \tilde{K} = \tilde{K} = 0 \), \( H_{E^{0},0} = 1 \), \( \tilde{L} = E^{e^{(i)}}_{E^{0} \text{sym}} \), \( c^e(E^{(i)}) = C_j \), and \( c(E^{e^{(i)})} = e^{(i)} \). Thus, each index-matrix \( E^{e^{(i)}}_{E^{0}} \) results in the term \( C_j \left[ \partial_j g(X) \right] \) in the \( L \)-sum. Summation of all the said terms results in multivariate Stein’s lemma, Eq. (4).

**Inductive hypothesis:** Eq. (5) holds true for \( n \).

**Inductive step:** Prove that Eq. (5) holds true for \( n + e^{(i)} \), \( i = 1, \ldots, N \). By using the inductive hypothesis, we have

\[
E \left[ g(X)X^{n+e^i} \right] = E \left[ (g(X)X^n)X^e \right] = \sum_{r(L) \leq n} \binom{n}{L} \mu^{n-r(L)} \sum_{K \leq K^{n-r(L)}} H_{L,K} \mathcal{C}_{L}^{L-K} E \left[ \partial^{L-K}(g(X)X^n) \right].
\]

(17)

By the general Leibniz rule [1, expression 3.3.8], we calculate the derivative

\[
\partial_i^{(L-K)} (g(X)X^n) = \sum_{p=0}^{c_i(L-K)} \binom{c_i(L-K)}{p} \partial_i^{(L-K-p)} g(X) \partial_p^{(L-K)} X^n.
\]

(18)

Since \( \partial_i^n X_i = X_i, \partial_i X_i = 1 \), and \( \partial_p^0 X_i = 0 \) for \( p \geq 2 \), Eq. (18) is simplified into

\[
\partial_i^{(L-K)} (g(X)X^n) = X_i \partial_i^{(L-K)} g(X) + c_i(L - K) \partial_i^{(L-K-1)} g(X) = X_i \partial_i^{(L-K)} g(X) + \sum_{j=1}^{N} \left[ \ell_{ji} - (1 + \delta_{ij})k_{ij} \right] \partial_i^{(L-K-1)} g(X),
\]

(19)

where \( \delta_{ij} \) is Kronecker’s delta. By using Eq. (19), we rewrite Eq. (17) as

\[
E \left[ (g(X)X^n)X^e \right] = A + \sum_{j=1}^{N} B_j,
\]

(20)

with

\[
A = \sum_{r(L) \leq n} \binom{n}{L} \mu^{n-r(L)} \sum_{K \leq K^{n-r(L)}} H_{L,K} \mathcal{C}_{L}^{L-K} E \left[ X_i \partial_i^{(L-K)} g(X) \right].
\]

(21)

and

\[
B_j = \sum_{r(L) \leq n} \binom{n}{L} \mu^{n-r(L)} \sum_{K \leq K^{n-r(L)}} \left[ \ell_{ji} - (1 + \delta_{ij})k_{ij} \right] H_{L,K} \mathcal{C}_{L}^{L-K} E \left[ \partial_i^{(L-K-1)} \prod_{p=1}^{N} \partial_p^{(L-K)} g(X) \right].
\]

(22)

In Eq. (22), the term in \( K \)-sum is zero for \( \ell_{ji} = 2k_{ij} \), or \( \ell_{ji} = k_{ij} \) for \( i \neq j \). In order to exclude zero terms, we update Eq. (22) to

\[
B_j = \sum_{r(L) \leq n} \binom{n}{L} \mu^{n-r(L)} \sum_{K \leq K^{n-r(L)} - E^{e^{(i)}}} \left[ \ell_{ji} - (1 + \delta_{ij})k_{ij} \right] H_{L,K} \mathcal{C}_{L}^{L-K} E \left[ \partial_i^{(L-K-1)} \prod_{p=1, p \neq i}^{N} \partial_p^{(L-K)} g(X) \right].
\]

(23)

By performing the change of index-matrix \( K' = K + E^{e^{(i)}}_{E^{0} \text{sym}} \), we recast Eq. (23) into

\[
B_j = \sum_{r(L) \leq n} \binom{n}{L} \mu^{n-r(L)} \sum_{K' \leq K^{\max}(L - E^{e^{(i)})} + E^{e^{(i)}}_{E^{0} \text{sym}}} \left[ \ell_{ji} - (1 + \delta_{ij})(k_{ij} - 1) \right] H_{L,K'} \mathcal{C}_{L}^{L-K'} \times E \left[ \partial_i^{(L-K')} \prod_{p=1}^{N} \partial_p^{(L-K')} g(X) \right].
\]

(24)
Since \( (\ell_{ij} - 1)/2 + 1 = ((\ell_{ij} + 1)/2) \), and \( \min(\ell_{ij}, \ell_{ji} - 1) = \min(\ell_{ij} + 1, \ell_{ji}) \) for \( i \neq j \), it holds true that \( K^{\max}(L - E^{(ij)}) + E^{(ij)}_{\text{sym}} = K^{\max}(L + E^{(ij)}) \). Thus, Eq. (24) is expressed equivalently as

\[
B_j = \sum_{r \in \mathbb{N}} \binom{n}{L} \sum_{k \leq K_{\text{sym}}(L + E^{(ij)})} \left( L_{ij} - (1 + \delta_{ij})(k_{ij} - 1) \right) H_{L,K} C_{L,K}^{L,K} \sum_{p=1}^{N} \left[ \delta_p^{(L-K)} \right] g(X).
\]

By applying Stein’s lemma (4) at the expectation appearing in the right-hand side of Eq. (21), we obtain

\[
A = A_0 + \sum_{j=1}^{N} A_j,
\]

with

\[
A_0 = \sum_{r \in \mathbb{N}} \binom{n}{L} \mu^{n-r(L)} \sum_{k \leq K_{\text{sym}}(L)} H_{L,K} C_{L,K}^{L,K} \left( \delta_p^{(L-K)} \right) g(X).
\]

and

\[
A_j = \sum_{r \in \mathbb{N}} \binom{n}{L} \mu^{n-r(L)} \sum_{k \leq K_{\text{sym}}(L)} H_{L,K} C_{L,K}^{L,K} \left( \delta_p^{(L-K)} \right) g(X).
\]

Thus, under Eqs. (20) and (26), the expectation is expressed as

\[
E \left[ (g(X)X_a)X^a \right] = A_0 + \sum_{j=1}^{N} (A_j + B_j).
\]

In order to evaluate each \( A_j + B_j \) further, we prove the following lemma.

**Lemma 1** (Recurrence relation for \( H_{L,K} \)). For \( L \in \mathbb{N}^{N \times N}, K \in \mathbb{N}^{N \times N} \) with \( 0 \leq K \leq K^{\max}(L + E^{(ij)}) \), and under the convention that \( H_{L,K} = 0 \) for \( K < 0 \) or \( K > K^{\max}(L) \), it holds true that

\[
H_{L,K} = H_{L,K} + [\ell_{ij} - (1 + \delta_{ij})(k_{ij} - 1)] H_{L,K} - E^{(ij)}_{\text{sym}}.
\]

**Proof.** See Appendix A. \( \square \)

Thus

\[
A_j + B_j = \sum_{r \in \mathbb{N}} \binom{n}{L} \mu^{n-r(L)} \sum_{k \leq K^{\max}(L + E^{(ij)})} H_{L,K} C_{L,K}^{L,K} E \left[ \delta_p^{(L-K)} \right] g(X).
\]

and by performing the index-matrix change \( L' = L + E^{(ij)} \)

\[
A_j + B_j = \sum_{r \in \mathbb{N}} \binom{n}{L} \mu^{n-r(L)} \sum_{k \leq K^{\max}(L')} H_{L,K} C_{L,K}^{L,K} E \left[ \delta_p^{(L-K)} \right] g(X).
\]

By also considering \( A_0 \) from Eq. (27), Eq. (29) reads

\[
E \left[ (g(X)X_a)X^a \right] = \sum_{r \in \mathbb{N}} \binom{n}{L} \sum_{j=1}^{N} \left( L - E^{(ij)} \right) \mu^{n-r(L)} \sum_{k \leq K_{\text{sym}}(L)} H_{L,K} C_{L,K}^{L,K} E \left[ \delta_p^{(L-K)} \right] g(X) +
\]

\[
+ \sum_{r \in \mathbb{N}} \binom{n}{L} \sum_{j=1}^{N} \left( L - E^{(ij)} \right) \mu^{n-r(L)} \sum_{k \leq K_{\text{sym}}(L)} H_{L,K} C_{L,K}^{L,K} E \left[ \delta_p^{(L-K)} \right] g(X).
\]

The inductive proof of Eq. (5) is completed by the following lemma.
Lemma 2 (Addition of $r$-multinomial coefficients). It holds true that
\[
\binom{n + e^{(i)}}{L}_r = \binom{n}{L}_r + \sum_{j=1}^{N} \binom{n}{L - E^{(j)}}_r, \text{ for } r(L) \leq n, \tag{34}
\]
\[
\binom{n + e^{(i)}}{L}_r = \sum_{j=1}^{N} \binom{n}{L - E^{(j)}}_r, \text{ for } r(L) = n + e^{(i)}. \tag{35}
\]

Proof. See Appendix B. □

Substitution of Eqs. (34), (35) into Eq. (33) results Eq. (5) for $n + e^{(i)}$.

3. Constructive formal derivation of theorem 1

Our alternative, constructive derivation of Eq. (5) is based on the following definition for the mean value operator.

Definition 1 (Mean value as the action of averaged shift operators). Let $X$ be an $N$-dimensional Gaussian random vector with mean value vector $\mu$ and autocovariance matrix $C$, and $g$ be a $C^\infty (\mathbb{R}^N \to \mathbb{R})$ function. The diagonal elements of matrix $C$ (the autocovariances of each $X_i$ component) are denoted as $\sigma_i^2 = C_{ii}$. The expectation $E \left[ g(X) \right]$ is expressed as
\[
E \left[ g(X) \right] = \left( \prod_{i=1}^{N} T_{ii} \right) \left( \prod_{j=1}^{N} \prod_{j=1}^{N} T_{ij} \right) g(\mu), \tag{36}
\]
where $T_{ij}$ are the pseudodifferential averaged shift operators defined as
\[
T_{ii} = \exp \left( \frac{\sigma_i^2}{2} \right), \quad i = 1, \ldots, N, \tag{37}
\]
\[
T_{ij} = \exp \left( C_{ij} \partial_i \partial_j \right), \quad i, j = 1, \ldots, N, \quad j \neq i, \tag{38}
\]
whose action is to be understood by their series forms
\[
T_{ii} = \sum_{m=0}^{\infty} \frac{\sigma_i^{2m}}{m!} \partial_i^{2m}, \quad i = 1, \ldots, N, \tag{39}
\]
\[
T_{ij} = \sum_{m=0}^{\infty} \frac{C_{ij}^{m}}{m!} \partial_i^m \partial_j^m, \quad i, j = 1, \ldots, N, \quad j \neq i. \tag{40}
\]

Proof. We formally derive Eq. (36) in Appendix C, using the moment-generating function of the $N$-dimensional Gaussian vector $X$. The infinite-dimensional counterpart of definition 1, regarding Gaussian processes, is presented in [2], and it is also found in [15, Ch. 4] as a concept. □

Remark 1 (Properties of $T_{ij}$ operators). Under the formal assumption that all infinite series involved are summable, and by employing the linearity of derivatives, we can easily see that $T_{ij}$ operators are linear, commute with differentiation operators $\partial_i$, and also commute with each other (see also [2, lemmata 1-3]).

Lemma 3 (Action of $T_{ii}$ operator). It holds true that
\[
T_{ii} \left[ g(x_i, \ldots, x_i) \right] = \sum_{\ell=0}^{n} \binom{n}{\ell} \prod_{k=0}^{\ell/2} H_{\ell/2} \sigma_i^{2(\ell-k)} T_{ii} \left[ \partial_i^{\ell-2k} g(x_i) \right], \tag{41}
\]
where $H_{\ell/2}$ are the signless Hermite coefficients, defined by Eq. (3).
Proof. See Appendix D. □

Lemma 4 (Action of $T_{ij}$, $j \neq i$ operator). It holds true that

$$ T_{ij} \left[ g(x)x_i^{n_i}x_j^{n_j} \right] = \sum_{l=0}^{n_i} \sum_{l'=0}^{n_j} \binom{n_i}{l} \binom{n_j}{l'} \sum_{k=0}^{\min(l, l')} G_{l, l', k} C_{ij}^l \left[ \delta_{i}^{l-k} \delta_{j}^{l'-k} g(x) \right], $$

with

$$ G_{l, l', k} = \binom{l_1}{k_1} \binom{l_2}{k_2} k!, \quad k = 0, \ldots, \min(l_1, l_2). $$

Similarly to $H_{l, k}$ coefficients, $G_{l, l', k}$'s are identified as the absolute values of the coefficients appearing in the 2-dimensional Itô–Hermite polynomials [11, 14].

Proof. See Appendix E. □

By expressing the expectation $E \left[ g(X) \left( \prod_{i=1}^{N} X_i^{n_i} \right) \right]$ via definition 1, we understand that, for its evaluation, it suffices to sequentially apply operators $T_{ij}$, $T_{ji}$, $i, j = 1, \ldots, N$, $j > i$ at the product $g(x) \left( \prod_{i=1}^{N} X_i^{n_i} \right)$, and set $x = \mu$ afterwards. After algebraic manipulations and using the operator properties of remark 1, we obtain

$$ E \left[ g(X) \left( \prod_{i=1}^{N} X_i^{n_i} \right) \right] = \sum_{m_{i}+\sum_{j=1}^{N} \ell_{j}=n_{j}} \left( N \prod_{i=1}^{N} \left( m_{i}, \ell_{i} \right) \right) \left( N^{m_{i}} \mu_{i} \right) \left( \prod_{i=1}^{N} H_{\ell_{i}, k_{i}} \partial_{i}^{2(l_{i}-k_{i})} \right) \times $$

$$ \times \left( \prod_{i=1}^{N} \prod_{j=1}^{N} G_{l_{i}, l_{j}, k_{i}, k_{j}} \partial_{i}^{l_{i}+l_{j}-k_{i}} \partial_{j}^{l_{j}+l_{i}-k_{j}} \right) E \left[ \prod_{i=1}^{N} \partial_{i}^{l_{i}+l_{j}-(1+k_{i}+k_{j})} g(X) \right], $$

with $k_{ij} = k_{ji}$. (44)

where $\binom{m_l}{n_{l}, \ell_{l_{i}} \cdots \ell_{l_{j}}} \frac{1}{m_{l}, l_{i} \cdots l_{j}}$ is the multinomial coefficient with $N+1$ factors. Sum $\sum_{m_{i}+\sum_{j=1}^{N} \ell_{j}=n_{j}}$ is over all combinations of integers $\{m_{i}, \ell_{i}, \ldots, \ell_{N}\}$. By recasting Eq. (44) into multi-index and index matrix notation, we obtain Eq. (5).

4. Conclusions and future works

In the present work, we derived formula (5) extending Stein’s lemma for the evaluation of $E \left[ g(X) \prod_{i=1}^{N} X_i^{n_i} \right]$, where $X$ is an $N$-dimensional Gaussian random vector. By our formula, the said expectation is expressed in terms of the expectations of partial derivatives of $g(X)$, as well as the mean value vector and autocovariance matrix of $X$. Furthermore, by setting $g(X) = 1$, formula (5) results in Isserlis theorem [13] and Song & Lee formula [31] for Gaussian product moments $E \left[ \prod_{i=1}^{N} X_i^{n_i} \right]$.

A direction for future works is the extension of the infinite-dimensional analog of Stein’s lemma, called the Novikov-Furutsu theorem (see [28, Sec. 11.5], [2]). In the infinite-dimensional case, $X$ is a Gaussian random process of time argument $t$, whose mean value is the function $\mu(t)$, and its two-time autocovariance function is $C(t_1, t_2)$. Thus, for $g$ being a functional of $X$ over the time interval $[t_0, t]$, Novikov-Furutsu theorem reads:

$$ E \left[ g[X] X(t) \right] = \mu(t) E \left[ g(X) \right] + \int_{t_0}^{t} C(t, s) E \left[ \frac{\delta g[X]}{\delta X(s)} \right] ds, $$

(45)

where $\delta g[X]/\delta X(s)$ is the Volterra functional derivative of $g[X]$ with respect to a local perturbation of process $X$ centered at time $s$ (see e.g. [2, Appendix A] for more on Volterra calculus). Novikov-Furutsu theorem, Eq. (45), is the main tool in deriving evolution equations, that resemble the classical Fokker-Planck equation, for the response probability density of dynamical systems under Gaussian random excitation, see e.g. [10, Eq.(3.19)], [20, 18]. Recently [19, Ch. 3], we extended Novikov-Furutsu theorem for expectations that contain the Gaussian argument at various times; $E \left[ g[X] \prod_{i=1}^{N} X(t_i) \right]$. As we have already shown in [2], the introduction and use of averaged shift operators is very helpful in constructing extensions of the Novikov-Furutsu theorem.
Appendix A. Proof of lemma 1

By using the definition relation (11), we easily calculate that

\[ H_{L+E(0)} = H_{L} = 1. \]  
(A.1)

Since, by convention, \( H_{L+E(0)} = 0 \), Eq. (A.1) coincides with recurrence relation (30) for \( K = 0 \). For \( L_{\text{sym}} \leq K \leq K_{\text{max}}(L) \), we have the following two cases.

First case: \( i = j \)

\[
H_{L,K} + (\ell_{ii} - 2k_{ii} + 2)H_{L,K-E_{ij}} = \\
\frac{2^N\sum_{\pi=1}^{m_p} k_{ij} \prod_{p=1}^{m_p} k_{pq}! \prod_{j=1}^{m_p} (k_{pq} - k_{ij})!}{L!} \left[ \frac{1}{2^{m} k_{ii}!(\ell_{ii} - 2k_{ii})!} + \frac{\ell_{ii} - 2k_{ii} + 2}{2^{m-1}(k_{ii} - 1)!(\ell_{ii} - 2k_{ii} + 2)!} \right] = \\
\frac{2^N\sum_{\pi=1}^{m_p} k_{ij} \prod_{p=1}^{m_p} k_{pq}! \prod_{j=1}^{m_p} (k_{pq} - k_{ij})!}{L!} \left[ \frac{\ell_{ij} + 1}{k_{ij}!(\ell_{ij} - k_{ij})!(\ell_{ij} - k_{ij})!} + \frac{\ell_{ij} - k_{ij} + 1}{(k_{ij} - 1)!(\ell_{ij} - k_{ij} + 1)!(\ell_{ij} - k_{ij} + 1)!} \right], 
(A.2)
\]

and since \( k_{ij} = k_{ji} \)

\[
H_{L,K} + (\ell_{ij} - k_{ij} + 1)H_{L,K-E_{ij}} = \\
\frac{2^N\sum_{\pi=1}^{m_p} k_{ij} \prod_{p=1}^{m_p} k_{pq}! \prod_{j=1}^{m_p} (k_{pq} - k_{ij})!}{L!} \left[ \frac{\ell_{ij} + 1}{k_{ij}!(\ell_{ij} - k_{ij})!(\ell_{ij} - k_{ij})!} + \frac{\ell_{ij} - k_{ij} + 1}{(k_{ij} - 1)!(\ell_{ij} - k_{ij} + 1)!(\ell_{ij} - k_{ij} + 1)!} \right]. 
(A.3)
\]

Last, we have to prove Eq. (30) for \( K = K_{\text{max}}(L + E^{(ij)}) \). Again, we distinguish two cases.

First case: \( i = j \). If \( \ell_{ii} \) is even, \( \lfloor \ell_{ii} / 2 \rfloor \leq \lfloor \ell_{ii} / 2 \rfloor \), and thus \( K_{\text{max}}(L + E^{(ij)}) = K_{\text{max}}(L) \). So, it remains to prove Eq. (30) for odd \( \ell_{ii} = 2a + 1 \) and for \( k_{ii} = k_{\text{max}}(L + E^{(ij)}) = \lfloor \ell_{ii} / 2 \rfloor = a + 1 \). In this case, we calculate

\[
\frac{H_{L,K_{\text{max}}(L+E^{(0)})}}{H_{L,K_{\text{max}}(L+E^{(0)})-E_{ij}}} = \frac{2^{2a+1} \prod_{r=1}^{2a+1} (l_{ii} - r + 1) (l_{ii} - r)!}{2^{2a+1} \prod_{r=1}^{2a+1} (l_{ii} - r + 1) (l_{ii} - r)!} = 1. 
(A.5)
\]

Since, by convention, \( H_{L,K_{\text{max}}(L+E^{(0)})} = 0 \) for this case, Eq. (A.5) is the specification of recurrence relation (30).

Second case: \( i \neq j \). If \( \ell_{ij} + 1 \geq \ell_{ji} \), \( K_{\text{max}}(L + E^{(ij)}) = K_{\text{max}}(L) \). Thus, it remains to prove Eq. (30) for \( \ell_{ij} + 1 < \ell_{ji} \), and for \( k_{ij} = k_{\text{max}}(L + E^{(ij)}) = \ell_{ij} + 1 \). In this case, we calculate

\[
\frac{H_{L,K_{\text{max}}(L+E^{(0)})}}{H_{L,K_{\text{max}}(L+E^{(0)})-E_{ij}}} = \frac{(l_{ij} + 1)!}{(l_{ji} + 1)! (l_{ij} - l_{ji} + 1)!} = \ell_{ij} - \ell_{ji}. 
(A.6)
\]

Since, by convention, \( H_{L,K_{\text{max}}(L+E^{(0)})} = 0 \) for this case, Eq. (A.6) is the specification of recurrence relation (30).
Appendix B. Proof of lemma 2

First case: \( r(L) \leq n \). Using the definition relation (10) for \( r \)-multinomial coefficients, we have

\[
\left( \frac{n}{L_r} \right) + \sum_{j=1}^{N} \left( \frac{n}{L - \mathbf{E}^{(j)}} \right) = \frac{n!}{[n - r(L)]!L!} + \sum_{j=1}^{N} \frac{n!}{[n - r(L - \mathbf{E}^{(j)})]!(L - \mathbf{E}^{(j)})!} = \frac{n!}{[n - r(L)]!L!} + \sum_{j=1}^{N} \frac{n!}{[n + \mathbf{E}^{(j)} - r(L)]!(L - \mathbf{E}^{(j)})!} = \frac{n!}{[n + \mathbf{E}^{(j)} - r(L)]!(L - \mathbf{E}^{(j)})!} \left[ n_i + 1 - r_i(L) + \sum_{j=1}^{N} \ell_{ij} \right] = \frac{[n + \mathbf{E}^{(j)}]!}{[n + \mathbf{E}^{(j)} - r(L)]!L!} \left( \frac{n + \mathbf{E}^{(j)}}{L} \right)_r. \tag{B.1}
\]

Second case: \( r(L) = n + \mathbf{E}^{(i)} \). Using the definition relation (10), we have

\[
\sum_{j=1}^{N} \left( \frac{n}{L - \mathbf{E}^{(j)}} \right) = \frac{n!}{[n + \mathbf{E}^{(j)} - r(L)]!(L - \mathbf{E}^{(j)})!} = \frac{n!}{[n + \mathbf{E}^{(j)} - r(L)]!(L - \mathbf{E}^{(j)})!} \sum_{j=1}^{N} \ell_{ij} = \frac{n!(n_i + 1)}{[n + \mathbf{E}^{(j)} - r(L)]!L!} = \frac{[n + \mathbf{E}^{(j)}]!}{[n + \mathbf{E}^{(j)} - r(L)]!L!} \left( \frac{n + \mathbf{E}^{(j)}}{L} \right)_r. \tag{B.2}
\]

Appendix C. Formal derivation of definition 1

The Taylor expansion of a \( C^\infty \left( \mathbb{R}^N \to \mathbb{R} \right) \) function \( g \) around \( x_0 \) is expressed via the shift pseudodifferential operator in exponential form (see e.g. [9, Sec. 1.1]) as

\[
g(x) = \left( 1 + \sum_{m=1}^{\infty} \frac{1}{m!} \sum_{n_1=1}^{N} \cdots \sum_{n_m=1}^{N} \hat{x}_{i_1} \cdots \hat{x}_{i_m} \partial_{i_1} \cdots \partial_{i_m} \right) g(x_0) = \left[ \sum_{m=0}^{\infty} \frac{1}{m!} \left( \sum_{i=1}^{N} \hat{x}_i \partial_i \right)^m \right] g(x_0) = \exp \left( \sum_{i=1}^{N} \hat{x}_i \partial_i \right) g(x_0), \tag{C.1}
\]

where \( \hat{x} = x - x_0 \) is called the shift argument. By substituting the random vector \( X \) as the argument of function \( g \), choosing \( x_0 = \mu \) where \( \mu \) is the mean value of \( X \), and taking the expectation in both sides of Eq. (C.1) results into

\[
\mathbb{E}[g(X)] = \mathbb{E} \left[ \exp \left( \sum_{i=1}^{N} \hat{X}_i \partial_i \right) \right] g(\mu) = M_\hat{g}(\nabla) g(\mu), \tag{C.2}
\]

where \( \hat{X} := X - \mu \) (the centered random vector) and \( \nabla = [\partial_1, \ldots, \partial_N]^T \) (the del vector). In Eq. (C.2), \( M_\hat{g}(u) \) is identified as the moment-generating function of \( \hat{X} \); \( M_\hat{g}(u) = \mathbb{E} \left[ \exp \left( u^T \hat{X} \right) \right] \), see [32, Sec. 4.3.3]. For the Gaussian vector \( X \) with autocovariance matrix \( \mathbf{C} \), the moment-generating function for the corresponding centered Gaussian random vector \( \hat{X} \) takes the form \( M_\hat{g}(u) = \exp \left( u^T \mathbf{C} u / 2 \right) \), see [32, Sec. 5.1.1]. Substitution of Gaussian \( M_\hat{g}(u) \) into Eq. (C.2) results in

\[
\mathbb{E}[g(X)] = \exp \left( \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} C_{ij} \partial_i \partial_j \right) g(\mu), \tag{C.3}
\]

and by using the symmetry property of autocovariance matrix \( \mathbf{C} \):

\[
\mathbb{E}[g(X)] = \exp \left( \sum_{i=1}^{N} \frac{\sigma_i^2}{2} \partial_i^2 + \sum_{i=1}^{N} \sum_{j=1}^{N} C_{ij} \partial_i \partial_j \right) g(\mu) = \left[ \prod_{i=1}^{N} \exp \left( \frac{\sigma_i^2}{2} \partial_i^2 \right) \right] \left[ \prod_{i=1}^{N} \prod_{j=1}^{N} \exp \left( C_{ij} \partial_i \partial_j \right) \right] g(\mu). \tag{C.4}
\]

Eq. (C.4) coincides with Eq. (36).
Appendix D. Proof of lemma 3

Expressing $T_u \left[ g(x)x_i^n \right]$ via Eq. (39) we have

$$T_u \left[ g(x)x_i^n \right] = \sum_{m=0}^{\infty} \sigma_i^{2m} \frac{2^{2m}}{2m!} \partial_i^{2m} \left( g(x) x_i^n \right). \quad \text{(D.1)}$$

The derivatives appearing in the right-hand side of Eq. (D.1) are further evaluated using the general Leibniz rule:

$$\partial_i^{2m} \left( g(x) x_i^n \right) = \sum_{\ell=0}^{2m} \frac{2m!}{\ell! \left( 2m-\ell \right)!} \partial_i^{2\ell} g(x) \partial_i^{2m-2\ell} \left( x_i^n \right). \quad \text{(D.2)}$$

Since $\partial_i^{\ell} x_i^n = (n!/(n-\ell)!)x_i^{n-\ell}$ for $n_i \geq \ell$ and zero for $n_i < \ell$, Eq. (D.2) is updated to

$$\partial_i^{2m} \left( g(x) x_i^n \right) = \sum_{\ell=0}^{\min \left[ m, 2m \right]} \frac{n_i!}{\ell! \left( 2m-\ell \right)!} \partial_i^{2\ell} g(x) \partial_i^{2m-2\ell} \left( x_i^n \right),$$

where $(2m)^\ell = (2m)(2m-1) \cdots (2m-\ell + 1)$ is the falling factorial. Substitution of Eq. (D.3) into Eq. (D.1) results in

$$T_u \left[ g(x)x_i^n \right] = \sum_{m=0}^{\infty} \min \left[ m, 2m \right] \sum_{\ell=0}^{\min \left[ m, 2m \right]} \frac{n_i!}{\ell! \left( 2m-\ell \right)!} \partial_i^{2\ell} \frac{(2m)^\ell}{2^m m!} \partial_i^{2m-2\ell} g(x). \quad \text{(D.4)}$$

In Eq. (D.4), the $m$ and $\ell$-summations are interchanged using formula (G.1), resulting into

$$T_u \left[ g(x)x_i^n \right] = \sum_{m=0}^{\infty} \sum_{\ell=0}^{\min \left[ m, 2m \right]} \frac{n_i!}{\ell! \left( 2m-\ell \right)!} \partial_i^{2\ell} \frac{(2m)^\ell}{2^m m!} \partial_i^{2m-2\ell} g(x). \quad \text{(D.5)}$$

Following [6, Sec. 8.4], see also [17, Eq.(30)], $(2m)^\ell$ is expressed in terms of $m^\ell$ as

$$\frac{(2m)^\ell}{2^m m!} = \sum_{p=\ell/2}^{\min \left[ m, 2m \right]} C(\ell, p; 2)m^p \quad \text{(D.6)}$$

where $C(\ell, p; 2)$ are the generalized factorial coefficients with parameter 2, and $\lceil \cdot \rceil$ is the ceiling function. Using also the fact $m^\ell m! = 1/(m-p)!$, Eq. (D.5) is expressed as

$$T_u \left[ g(x)x_i^n \right] = \sum_{m=0}^{\infty} \sum_{\ell=0}^{\min \left[ m, 2m \right]} \frac{n_i!}{\ell! \left( 2m-\ell \right)!} \partial_i^{2\ell} \frac{C(\ell, p; 2)}{(m-p)!} \partial_i^{2m-2\ell} g(x). \quad \text{(D.7)}$$

By also interchanging the $m$ and $p$-summations using formula (G.7), we have

$$T_u \left[ g(x)x_i^n \right] = \sum_{\ell=0}^{n_i} \left( \frac{n_i}{\ell} \right) x_i^{n_i-\ell} \sum_{\ell=0}^{\min \left[ m, 2m \right]} \sum_{p=\ell/2}^{\min \left[ m, 2m \right]} \frac{C(\ell, p; 2)}{(m-p)!} \partial_i^{2m-2\ell} g(x). \quad \text{(D.8)}$$

An index change in the $m$-sum, and the use of Eq. (39), results in

$$T_u \left[ g(x)x_i^n \right] = \sum_{\ell=0}^{n_i} \left( \frac{n_i}{\ell} \right) x_i^{n_i-\ell} \sum_{p=\ell/2}^{\min \left[ m, 2m \right]} \frac{C(\ell, p; 2)}{(m-p)!} \partial_i^{2m-2p} \partial_i^{2m-2p} g(x) = \sum_{\ell=0}^{n_i} \left( \frac{n_i}{\ell} \right) x_i^{n_i-\ell} \sum_{p=\ell/2}^{\min \left[ m, 2m \right]} \frac{C(\ell, p; 2)}{(m-p)!} \partial_i^{2m-2p} g(x). \quad \text{(D.9)}$$
As we have showed in the recent work \[m\] Hermite polynomials, see \[m\] Substitution of Eq. \((E.4)\), we have

\[
\mathcal{T}_{ij} \left[ g(x) x_i^{n_j} x_j^{n_j} \right] = \sum_{m=0}^{\infty} \sum_{i=0}^{\min\{m,m\}} \frac{C_m^m}{m!} \partial_{x_j}^m \partial_{x_i}^m \left( g(x) x_i^{n_j} x_j^{n_j} \right).
\] (E.1)

As in Appendix D, the derivatives \(\partial_{x_j}^m, \partial_{x_i}^m\) in the right-hand side of Eq. \((E.1)\) can be evaluated further using general Leibniz rule, resulting in

\[
\mathcal{T}_{ij} \left[ g(x) x_i^{n_j} x_j^{n_j} \right] = \sum_{m=0}^{\infty} \sum_{i=0}^{\min\{m,m\}} \left( \frac{C_m^m}{m!} \partial_{x_j}^m \partial_{x_i}^m \left( g(x) x_i^{n_j} x_j^{n_j} \right) \right).
\] (E.2)

By rearranging the summations in Eq. \((E.2)\) using formula \((G.10)\), we obtain

\[
\mathcal{T}_{ij} \left[ g(x) x_i^{n_j} x_j^{n_j} \right] = \sum_{i=0}^{\min\{m,m\}} \sum_{j=0}^{\min\{m,m\}} \left( \frac{C_m^m}{m!} \partial_{x_j}^m \partial_{x_i}^m \left( g(x) x_i^{n_j} x_j^{n_j} \right) \right).
\] (E.3)

In order to evaluate the right-hand side of Eq. \((E.3)\) further, the product of the two falling factorials \(n_j^m n_i^m\) has to be expressed in terms of falling factorials of \(m\). This is performed by the following lemma.

**Lemma 5** (Product of two falling factorials of \(m\)). It holds true that

\[
m_i^m m_j^m = \sum_{k=0}^{\min\{m,m\}} G_{\ell,\ell,k} m_{\ell+k}^{\ell+k}
\] (E.4)

**Proof.** See Appendix F. \(\square\)

Since, by the definition of falling factorial, \(m_{\ell+k}^{\ell+k}\) is zero for \(\ell_i + \ell_j - k > m\), Eq. \((E.4)\) is updated to

\[
m_i^m m_j^m = \sum_{k=\max\{0,\ell_i,\ell_j\}}^{\min\{m,m\}} G_{\ell,\ell,k} m_{\ell+k}^{\ell+k}
\] (E.5)

Substitution of Eq. \((E.5)\) into Eq. \((E.3)\), and use of \(m_{\ell_i \ell_j - k} / m! = 1/(m - \ell_i - \ell_j + k)!\) results in

\[
\mathcal{T}_{ij} \left[ g(x) x_i^{n_j} x_j^{n_j} \right] = \sum_{i=0}^{\min\{m,m\}} \sum_{j=0}^{\min\{m,m\}} \sum_{k=\max\{0,\ell_i,\ell_j\}}^{\min\{m,m\}} \sum_{m=\max\{0,\ell_i,\ell_j\}}^{\min\{m,m\}} \frac{C_m^m}{m!} G_{\ell_i \ell_j, k} \partial_{\ell_i}^m \partial_{\ell_j}^m g(x).
\] (E.6)

By interchanging \(m\) and \(k\)-summations using formula \((G.15)\), we have

\[
\mathcal{T}_{ij} \left[ g(x) x_i^{n_j} x_j^{n_j} \right] = \sum_{i=0}^{\min\{m,m\}} \sum_{j=0}^{\min\{m,m\}} \sum_{k=0}^{\min\{m,m\}} \sum_{m=\ell_i + \ell_j + k}^{\min\{m,m\}} \frac{C_m^m}{m!} G_{\ell_i \ell_j, k} \partial_{\ell_i}^m \partial_{\ell_j}^m g(x).
\] (E.7)
An index change in the \( m \)-sum results in
\[
T_{ij} [g(x) x_i^{n_i} x_j^{n_j}] = \sum_{\ell_0}^{n_i} \sum_{\ell_j}^{n_j} \left[ \sum_{\ell_k}^{\min(\ell_i, \ell_j)} \binom{m}{\ell_k} x_i^{\ell_i-\ell_k} x_j^{\ell_j-\ell_k} \right] G_{\ell_i, \ell_j, k} \sum_{m=0}^{\infty} \sum_{k=0}^{\infty} C_{ij}^{m} d_j^{m+\ell_j-k} d_i^{m+\ell_i-k} g(x).
\] (E.8)

Eq. (E.8), by virtue of Eq. (40), coincides with Eq. (42).

Appendix F. Proof of lemma 5

Our starting point for proving Eq. (E.4) is Vandermonde’s identity (see e.g. [6, example 3.6])
\[
\binom{m}{\ell_i + \ell_j} = \sum_{k=0}^{\ell_i} \binom{m}{k} \binom{m-k}{\ell_i-k} \tag{F.1}
\]

By multiplying both sides of Eq. (F.1) by \( \binom{m}{\ell_i} \), and after some algebraic manipulations, we obtain
\[
\binom{m}{\ell_i} \binom{m}{\ell_j} = \sum_{k=0}^{\ell_i} \binom{m}{k} \binom{m-k}{\ell_i-k} \binom{m}{\ell_i + \ell_j - k} = \sum_{k=0}^{\ell_i} \binom{\ell_i}{k} \binom{\ell_j}{\ell_i - k} \binom{m}{\ell_i + \ell_j - k}. \tag{F.2}
\]

Since \( \binom{\ell_i + \ell_j - k}{k, \ell_i - k, \ell_j - k} \) = 0 for \( k > \ell_i \) or \( k > \ell_j \), upper limit of \( k \)-sum in Eq. (F.2) is updated to \( \min(\ell_i, \ell_j) \). By also using the fact that \( m^k = \binom{m}{0} k! \), see [6, Eq. (3.11)], Eq. (F.2) results in
\[
m^{\ell_i + \ell_j} = \sum_{k=0}^{\min(\ell_i, \ell_j)} G_{\ell_i, \ell_j, k} m^{\ell_i + \ell_j - k}, \tag{F.3}
\]

where
\[
G_{\ell_i, \ell_j, k} = \binom{\ell_i + \ell_j - k}{\ell_i - k, \ell_j - k} \binom{\ell_i! \ell_j!}{\ell_i + \ell_j - k}! \binom{\ell_i}{k} \binom{\ell_j}{\ell_i - k}!.
\]

Eq. (F.3) coincides with Eq. (E.4), and Eq. (F.4) coincides with the definition relation (43) of \( G_{\ell_i, \ell_j, k} \), completing thus the proof of lemma 5.

Appendix G. Summation rearrangement formulas and their proofs

In this Appendix, we prove the formulas (G.1), (G.7), (G.10), (G.15) rearranging multiple summations, that are employed in Appendices Appendix D, Appendix E for the proofs of lemmata 3, 4 respectively.

\[
\sum_{m=0}^{\infty} \sum_{\ell=0}^{\min(n, 2m)} A_{m, \ell} = \sum_{m=0}^{n} \sum_{\ell=0}^{\ell/2 \min(\ell/2)} A_{m, \ell}. \tag{G.1}
\]

**Proof.** We distinguish the cases of even and odd \( n \). For \( n = 2p \), the left-hand side of Eq. (G.1) is split into

\[
\sum_{m=0}^{\infty} \sum_{\ell=0}^{2p} A_{m, \ell} = \sum_{m=0}^{p} \sum_{\ell=0}^{2m} A_{m, \ell} + \sum_{m=p+1}^{2p} \sum_{\ell=0}^{\ell/2} A_{m, \ell}. \tag{G.2}
\]

In the right-hand side of Eq. (G.2), the sums of the second term are interchanged. The double summation of the first term is over the triangle \( 0 \leq m \leq p, 0 \leq \ell \leq 2m \) which is rearranged into \( 0 \leq \ell \leq 2p, \ell/2 \leq m \leq p \) and since \( m, \ell \) are integers; \( 0 \leq \ell \leq 2p, \ell/2 \leq m \leq p \). Thus:

\[
\sum_{m=0}^{\infty} \sum_{\ell=0}^{2p} A_{m, \ell} = \sum_{\ell=0}^{2p} \sum_{m=\ell/2}^{p} A_{m, \ell} + \sum_{m=\ell/2}^{2p} \sum_{\ell=0}^{2p} A_{m, \ell} = \sum_{\ell=0}^{2p} \sum_{m=\ell/2}^{2p} A_{m, \ell}. \tag{G.3}
\]
For \( n = 2p + 1 \), the left-hand side of Eq. (G.1) is split into
\[
\sum_{m=0}^{\infty} \sum_{\ell=0}^{\min(2p+1,2m)} A_{m,\ell} = \sum_{m=0}^{p} \sum_{\ell=0}^{2m} A_{m,\ell} + \sum_{m=p+1}^{\infty} \sum_{\ell=0}^{2p+1} A_{m,\ell} = \sum_{m=0}^{p} \sum_{\ell=0}^{2m} A_{m,\ell} + \sum_{m=p+1}^{\infty} \sum_{\ell=0}^{2p+1} A_{m,\ell} + \sum_{m=p+1}^{\infty} A_{m,2p+1}.
\] (G.4)

In the rightmost side of Eq. (G.4), the double summations are rearranged as for Eq. (G.2), resulting into
\[
\sum_{m=0}^{\infty} \sum_{\ell=0}^{\min(2p+1,2m)} A_{m,\ell} = \sum_{m=0}^{\infty} \sum_{\ell=0}^{\max(2p+1,2m)} A_{m,\ell}.
\] (G.5)

Since \( p + 1 = \lceil (2p + 1)/2 \rceil \), we identify the single sum in the right-hand side of Eq. (G.5) as the \( \ell = 2p + 1 \) term of the double sum:
\[
\sum_{m=0}^{\infty} \sum_{\ell=0}^{\min(2p+1,2m)} A_{m,\ell} = \sum_{m=0}^{\infty} \sum_{\ell=0}^{\max(2p+1,2m)} A_{m,\ell}.
\] (G.6)

Thus, the proof of Eq. (G.1) for both even and odd \( n \) is completed. \( \square \)

**Proof.** The left-hand side of Eq. (G.7) is split into
\[
\sum_{m=n}^{\infty} \sum_{k=\min(f,m)} A_{m,k} = \sum_{k=n}^{\infty} \sum_{m=\min(k,f)} A_{m,k}.
\] (G.7)

In the right-hand side of Eq. (G.8), the sums of the second term are interchanged. The double summation of the first term is over the triangle \( n \leq m \leq \ell, n \leq k \leq m \) which is rearranged into \( n \leq k \leq \ell, k \leq m \leq \ell \). Thus:
\[
\sum_{m=n}^{\infty} \sum_{k=\min(f,m)} A_{m,k} = \sum_{k=n}^{\ell} \sum_{m=\min(k,f)} A_{m,k} = \sum_{k=n}^{\ell} \sum_{m=\min(k,f)} A_{m,k},
\] (G.9)

which completes the proof of Eq. (G.7). \( \square \)

**Proof.** Without loss of generality, we assume that \( n_1 < n_2 \). Then, the left-hand side of Eq. (G.10) is split into
\[
\sum_{m=0}^{\infty} \sum_{\ell_1=0}^{\min(n_1,m)} \sum_{\ell_2=0}^{\min(n_2,m)} A_{m,\ell_1,\ell_2} = \sum_{m=0}^{n_1} \sum_{\ell_1=0}^{m} \sum_{\ell_2=0}^{m} A_{m,\ell_1,\ell_2} + \sum_{m=n_1+1}^{\infty} \sum_{\ell_1=0}^{m} \sum_{\ell_2=0}^{m} A_{m,\ell_1,\ell_2} + \sum_{m=n_2+1}^{\infty} \sum_{\ell_1=0}^{m} \sum_{\ell_2=0}^{m} A_{m,\ell_1,\ell_2}.
\] (G.11)

In the first term of the right-hand side of Eq. (G.11), the summation is over \( 0 \leq m \leq n_1, 0 \leq \ell_1 \leq m, 0 \leq \ell_2 \leq m \), which can be rearranged into \( 0 \leq \ell_1 \leq n_1, 0 \leq \ell_2 \leq n_1 \), \( \max(\ell_1,\ell_2) \leq m \leq n_1 \). In the second term, the summation over \( n_1 + 1 \leq m \leq n_2, 0 \leq \ell_2 \leq m \) is rearranged into \( 0 \leq \ell_2 \leq n_2, \max(n_1 + 1,\ell_2) \leq m \leq n_2 \). Thus, Eq. (G.11) is expressed equivalently as
\[
\sum_{m=0}^{\infty} \sum_{\ell_1=0}^{\min(n_1,m)} \sum_{\ell_2=0}^{\min(n_2,m)} A_{m,\ell_1,\ell_2} = \sum_{\ell_1=0}^{n_1} \sum_{\ell_2=0}^{n_1} \sum_{m=\max(\ell_1,\ell_2)}^{n_1} A_{m,\ell_1,\ell_2} + \sum_{\ell_1=0}^{n_1} \sum_{\ell_2=0}^{n_2} \sum_{m=\max(\ell_1,\ell_2)}^{n_1} A_{m,\ell_1,\ell_2} + \sum_{\ell_1=0}^{n_2} \sum_{\ell_2=0}^{n_2} \sum_{m=\max(\ell_1,\ell_2)}^{n_1} A_{m,\ell_1,\ell_2}.
\] (G.12)
The second term in the right-hand side of Eq. (G.12) is regrouped as

\[
\sum_{\ell_1=0}^{n_1} \sum_{\ell_2=0}^{n_2} \sum_{m=\max(n_1+1,\ell_2)}^{\min(n_1, m)} A_{m,\ell_1,\ell_2} = \sum_{\ell_1=0}^{n_1} \sum_{\ell_2=0}^{n_2} \sum_{m=\max(\ell_2+1, n_1+1)}^{\min(n_1, m)} A_{m,\ell_1,\ell_2} + \sum_{\ell_1=0}^{n_1} \sum_{\ell_2=0}^{n_2} \sum_{m=\max(\ell_2+1, n_1+1)}^{n_2} A_{m,\ell_1,\ell_2} = \sum_{\ell_1=0}^{n_1} \sum_{\ell_2=0}^{n_2} \sum_{m=\max(\ell_2+1, n_1+1)}^{\min(n_1, m)} A_{m,\ell_1,\ell_2} + \sum_{\ell_1=0}^{n_1} \sum_{\ell_2=0}^{n_2} \sum_{m=\max(\ell_2+1, n_1+1)}^{n_2} A_{m,\ell_1,\ell_2} + \sum_{\ell_1=0}^{n_1} \sum_{\ell_2=0}^{n_2} \sum_{m=\max(\ell_2+1, n_1+1)}^{\min(n_1, m)} A_{m,\ell_1,\ell_2}.
\]

Substitution of Eq. (G.13) into Eq. (G.12) results in

\[
\sum_{m=0}^{\infty} \sum_{\ell_1=0}^{\min(n_1, m)} \sum_{\ell_2=0}^{\min(n_2, m)} A_{m,\ell_1,\ell_2} = \sum_{\ell_1=0}^{n_1} \sum_{\ell_2=0}^{n_2} \sum_{m=\max(\ell_2+1, n_1+1)}^{\min(n_1, m)} A_{m,\ell_1,\ell_2} + \sum_{\ell_1=0}^{n_1} \sum_{\ell_2=0}^{n_2} \sum_{m=\max(\ell_2+1, n_1+1)}^{n_2} A_{m,\ell_1,\ell_2} + \sum_{\ell_1=0}^{n_1} \sum_{\ell_2=0}^{n_2} \sum_{m=\max(\ell_2+1, n_1+1)}^{\min(n_1, m)} A_{m,\ell_1,\ell_2},
\]

which coincides with Eq. (G.10).

**Proof.** Without the loss of generality, we assume that \( \ell_1 < \ell_2 \). Thus, Eq. (G.15) is simplified into

\[
\sum_{m=\max(\ell_1+\ell_2, 0)}^{\infty} \sum_{k=0}^{\min(\ell_1, \ell_2)} A_{m,k} = \sum_{m=\max(\ell_1+\ell_2, 0)}^{\infty} \sum_{k=0}^{\min(\ell_1, \ell_2)} A_{m,k}.
\]

Then, the left-hand side of Eq. (G.16) is split into

\[
\sum_{m=\max(\ell_1+\ell_2, 0)}^{\infty} \sum_{k=0}^{\min(\ell_1, \ell_2)} A_{m,k} = \sum_{m=\max(\ell_1+\ell_2, 0)}^{\infty} \sum_{k=0}^{\min(\ell_1, \ell_2)} A_{m,k} + \sum_{m=\max(\ell_1+\ell_2, 0)}^{\infty} \sum_{k=0}^{\min(\ell_1, \ell_2)} A_{m,k}.
\]

In the right-hand side of Eq. (G.17), the sums of the second term are interchanged. The double summation of the first term is over the triangle \( \ell_2 \leq m \leq \ell_1 + \ell_2, \ell_1 + \ell_2 - m \leq k \leq \ell_1 \) which is rearranged into \( 0 \leq k \leq \ell_1 \), \( \ell_1 + \ell_2 - k \leq m \leq \ell_1 + \ell_2 \). Thus:

\[
\sum_{m=\max(\ell_1+\ell_2, 0)}^{\infty} \sum_{k=0}^{\min(\ell_1, \ell_2)} A_{m,k} = \sum_{k=0}^{\min(\ell_1, \ell_2)} \sum_{m=\max(\ell_1+\ell_2, 0)}^{\infty} A_{m,k} + \sum_{k=0}^{\min(\ell_1, \ell_2)} \sum_{m=\max(\ell_1+\ell_2, 0)}^{\infty} A_{m,k}.
\]

which coincides with Eq. (G.16).

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