Fock space algebraic methods: Normal ordering with respect to Ψ

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1 Moments and cumulants

Note: In this section, sums $\sum_n$ without specified ranges should be taken to run from 1 to ∞.

1.1 Moments and cumulants in classical statistics

Definition 1.1. ***Moments of commuting random variables.*** Given a set $\{q_i\}$ of commuting random variables, their *moments* $\gamma(q_{i_1}\cdots q_{i_n})$ are defined as

$$\gamma(q_{i_1}\cdots q_{i_n}) = \langle q_{i_1}\cdots q_{i_n}\rangle \tag{1.1}$$

where $\langle X\rangle$ represents an expecation value $\mathbb{E}(X)$.

Remark 1.1. ***Expectation values from moments.*** Given a complete set of moments $\{\gamma(q_{i_1}\cdots q_{i_n})\}$, the expectation value of any analytic function $f(q_i)$ of the random variables can be obtained as

$$\langle f(q_i)\rangle = f(0) + \sum_n \frac{1}{n!}\sum_{i_1\cdots i_n} \left.\frac{\partial^n f}{\partial q_{i_1}\cdots\partial q_{i_n}}\right|_{q_i=0} \gamma(q_{i_1}\cdots q_{i_n}) \tag{1.2}$$

which results from expanding $f(q_i)$ in a Taylor series, noting that the expectation value is linear, and applying Def 1.1.

Definition 1.2. ***Moment and cumulant generating functions of commuting random variables.*** Given a set $\{q_i\}$ of commuting random variables, its *moment-generating function*, $M(\boldsymbol{\alpha})$, and its *cumulant-generating function*, $K(\boldsymbol{\alpha})$, are defined as

$$M(\boldsymbol{\alpha}) \equiv \langle e^{\sum_i \alpha_i q_i}\rangle \qquad M(\boldsymbol{\alpha}) = 1 + \sum_n \sum_{i_1\cdots i_n} \frac{\alpha_{i_1}\cdots\alpha_{i_n}}{n!}\gamma(q_{i_1}\cdots q_{i_n}) \tag{1.3}$$

$$K(\boldsymbol{\alpha}) \equiv \ln M(\boldsymbol{\alpha}) = \ln\langle e^{\sum_i \alpha_i q_i}\rangle \qquad K(\boldsymbol{\alpha}) = 0 + \sum_n \sum_{i_1\cdots i_n} \frac{\alpha_{i_1}\cdots\alpha_{i_n}}{n!}\lambda(q_{i_1}\cdots q_{i_n}) \tag{1.4}$$

where $\gamma(q_{i_1}\cdots q_{i_n})$ and $\lambda(q_{i_1}\cdots q_{i_n})$ are (respectively) the *moments* and *cumulants* that they generate. The moments and cumulants are obtained from $M(\boldsymbol{\alpha})$ and $K(\boldsymbol{\alpha})$ via

$$\gamma(q_{i_1}\cdots q_{i_n}) \equiv \left.\frac{\partial^n M(\boldsymbol{\alpha})}{\partial\alpha_{i_1}\cdots\partial\alpha_{i_n}}\right|_{\boldsymbol{\alpha}=0} \qquad \lambda(q_{i_1}\cdots q_{i_n}) \equiv \left.\frac{\partial^n K(\boldsymbol{\alpha})}{\partial\alpha_{i_1}\cdots\partial\alpha_{i_n}}\right|_{\boldsymbol{\alpha}=0} \tag{1.5}$$

as can be seen from equations 1.3 and 1.4.

Proposition 1.1. ***Moment-cumulant relations of commuting random variables.*** *The moments and cumulants of a set $\{q_i\}$ of commuting random variables are related via*

$$\gamma(q_{i_1}\cdots q_{i_n}) = \sum_{k=1}^{n} \sum_{(Q_1\cdots Q_k)}^{\mathcal{P}_k(q_{i_1}\cdots q_{i_n})} \lambda(Q_1)\cdots\lambda(Q_k) \tag{1.6}$$

$$\lambda(q_{i_1}\cdots q_{i_n}) = \sum_{k=1}^{n} (-)^{k+1}(k-1)! \sum_{(Q_1\cdots Q_k)}^{\mathcal{P}_k(q_{i_1}\cdots q_{i_n})} \gamma(Q_1)\cdots\gamma(Q_k) \tag{1.7}$$

where $(Q_1, \dots, Q_k) \in \mathcal{P}_k(q_{i_1} \cdots q_{i_n})$ *are unique* k*-tuple partitions of the product* $q_{i_1} \cdots q_{i_n}$*.*[1]
Proof: See Prop A.1.

1.2 Moments and cumulants of particle-hole operators

Remark 1.2. ***Motivating the form of*** $M(\boldsymbol{\alpha})$ ***for particle-hole operators.*** Just as the expectation value of a function of classical random variables can be obtained from its moment expansion (see Rmk 1.1), the expectation value of an m-electron Fock space operator (see **??**) can be obtained as

$$\langle \Psi | \boldsymbol{\Omega}(q_i) | \Psi \rangle = \frac{1}{m!} \sum_{\substack{p_1 \cdots p_m \\ q_1 \cdots q_m}} \Omega^{q_1 \cdots q_m}_{p_1 \cdots p_m} \ \gamma(a^\dagger_{p_1} \cdots a^\dagger_{p_m} a_{q_m} \cdots a_{q_1})$$

where $\gamma(a^\dagger_{p_1} \cdots a^\dagger_{p_m} a_{q_m} \cdots a_{q_1}) = \langle \Psi | a^\dagger_{p_1} \cdots a^\dagger_{p_m} a_{q_m} \cdots a_{q_1} | \Psi \rangle$ is a moment of the particle-hole operators (also known as an *m-particle reduced density matrix*). In particular, the electronic energy can be obtained from $\gamma(a^\dagger_p a_q)$ and $\gamma(a^\dagger_p a^\dagger_q a_s a_r)$ as

$$E_e = \langle \Psi | H_e(q_i) | \Psi \rangle = \sum_{pq} h^q_p \gamma(a^\dagger_p a_q) + \frac{1}{2} \sum_{pqrs} g^{rs}_{pq} \gamma(a^\dagger_p a^\dagger_q a_s a_r) \ .$$

However, the derivatives of $\langle \Psi | e^{\sum_i \alpha_i q_i} | \Psi \rangle$ do not generate these moments because the q_i do not commute. Noting that the operator products defining m-electron Fock space operators are in vac-normal order, we can generate the moments we need by normal-ordering the exponential in the moment generating function.

$$M(\boldsymbol{\alpha}) \equiv \langle \Psi | \boldsymbol{:} e^{\sum_i \alpha_i q_i} \boldsymbol{:} | \Psi \rangle = 1 + \sum_n \sum_{i_1 \cdots i_n} \frac{\alpha_{i_1} \cdots \alpha_{i_n}}{n!} \langle \Psi | \boldsymbol{:} q_{i_1} \cdots a_{i_n} \boldsymbol{:} | \Psi \rangle \tag{1.8}$$

However, the relation

$$\frac{\partial^n M(\boldsymbol{\alpha})}{\partial \alpha_{i_1} \cdots \partial \alpha_{i_n}} = \langle \Psi | \boldsymbol{:} q_{i_1} \cdots q_{i_n} \boldsymbol{:} | \Psi \rangle \tag{1.9}$$

does not hold if we take $\boldsymbol{\alpha}$ to consist of ordinary $\mathbb{C}$-numbers (the derivative will actually be 0 if $\alpha_i \in \mathbb{C}$). In fact, since $\boldsymbol{:} q_{i_1} \cdots q_{i_n} \boldsymbol{:}$ is antisymmetric with respect to permutations of $i_1 \cdots i_n$, equation 1.9 requires

$$\frac{\partial^n M(\boldsymbol{\alpha})}{\partial \alpha_{i_1} \cdots \partial \alpha_{i_n}} = \varepsilon_\pi \frac{\partial^n M(\boldsymbol{\alpha})}{\partial \alpha_{i_{\pi(1)}} \cdots \partial \alpha_{i_{\pi(n)}}}$$

for consistency, i.e. the probe variable derivatives must anticommute. This is a known property of so-called *Grassmann numbers*, which are "anticommuting numbers" frequently used in studying the statistics of Fermions. (See Cahill and Glauber, *Phys. Rev. A*, **59**, 1538 (1999) for more details).

Definition 1.3. ***Grassmann numbers.*** A system of particle-hole operators $\{q_i\}$ can be associated with a set of *Grassmann numbers* which are defined to satisfy $[\alpha_i, \alpha_j]_+ = [\alpha_i, q_j]_+ = 0$, i.e. they anticommute among themselves and with all particle-hole operators. Consistency demands that derivatives with respect to Grassmann-valued variables also anticommute, i.e. $\left[\frac{\partial}{\partial \alpha_i}, \frac{\partial}{\partial \alpha_j}\right]_+ = 0$, so that $\frac{\partial}{\partial \alpha_i} \frac{\partial}{\partial \alpha_j} \alpha_j \alpha_i = \frac{\partial}{\partial \alpha_i} \alpha_i = 1$.

Definition 1.4. ***Moments of particle-hole operators.*** Given a set $\{q_i\}$ of particle-hole operators, their *moments* $\gamma(q_{i_1} \cdots q_{i_n})$ are defined as

$$\gamma(q_{i_1} \cdots q_{i_n}) \equiv \langle \Psi | \boldsymbol{:} q_{i_1} \cdots a_{i_n} \boldsymbol{:} | \Psi \rangle \tag{1.10}$$

for a given state Ψ and ordering $\boldsymbol{::}$.

Definition 1.5. ***Moment and cumulant generating functions of particle-hole operators.*** The *moment-generating function*, $M(\boldsymbol{\alpha})$, and *cumulant-generating function*, $K(\boldsymbol{\alpha})$, of a set $\{q_i\}$ of particle-hole operators is given by

$$M(\boldsymbol{\alpha}) \equiv \langle \Psi | \boldsymbol{:} e^{\sum_i \alpha_i q_i} \boldsymbol{:} | \Psi \rangle \qquad M(\boldsymbol{\alpha}) = 1 + \sum_n \sum_{i_1 \cdots i_n} \frac{\alpha_{i_1} \cdots \alpha_{i_n}}{n!} \gamma(q_{i_1} \cdots q_{i_n}) \tag{1.11}$$

$$K(\boldsymbol{\alpha}) \equiv \ln M(\boldsymbol{\alpha}) = \ln \langle \Psi | \boldsymbol{:} e^{\sum_i \alpha_i q_i} \boldsymbol{:} | \Psi \rangle \qquad K(\boldsymbol{\alpha}) = 0 + \sum_n \sum_{i_1 \cdots i_n} \frac{\alpha_{i_1} \cdots \alpha_{i_n}}{n!} \lambda(q_{i_1} \cdots q_{i_n}) \tag{1.12}$$

[1] These "product partitions" are simply set partitions with each set of operators mapped to their product.

where $\{\alpha_i\}$ consists of Grassmann variables and $\mathbf{::}$ indicates vac-normal ordering. Moments and cumulants are given by

$$\gamma(q_{i_1}\cdots q_{i_n}) \equiv \left.\frac{\partial^n M(\boldsymbol{\alpha})}{\partial\alpha_{i_n}\cdots\partial\alpha_{i_1}}\right|_{\boldsymbol{\alpha}=0} \qquad \lambda(q_{i_1}\cdots q_{i_n}) \equiv \left.\frac{\partial^n K(\boldsymbol{\alpha})}{\partial\alpha_{i_n}\cdots\partial\alpha_{i_1}}\right|_{\boldsymbol{\alpha}=0} \tag{1.13}$$

where the ordering of partial derivatives has been chosen to yield the correct phase.

Proposition 1.2. ***Moment-cumulant relations of particle-hole operators.*** *The moments and cumulants of a set $\{q_i\}$ of particle-hole operators are related via*

$$\gamma(q_{i_1}\cdots q_{i_n}) = \sum_{k=1}^{n}\sum_{(Q_1\cdots Q_k)}^{\mathcal{P}_k(q_{i_1}\cdots q_{i_n})}(-)^{n_{\mathbf{Q}}}\lambda(Q_1)\cdots\lambda(Q_k) \tag{1.14}$$

$$\lambda(q_{i_1}\cdots q_{i_n}) = \sum_{k=1}^{n}(-)^{k+1}(k-1)!\sum_{(Q_1\cdots Q_k)}^{\mathcal{P}_k(q_{i_1}\cdots q_{i_n})}(-)^{n_{\mathbf{Q}}}\gamma(Q_1)\cdots\gamma(Q_k) \tag{1.15}$$

where $(Q_1,\ldots,Q_k)\in\mathcal{P}_k(q_{i_1}\cdots q_{i_n})$ are unique k-tuple partitions of the product $q_{i_1}\cdots q_{i_n}$. The operators within each block Q_i of the partition are taken to appear in the same order as they do in the original product, and $n_{\mathbf{Q}}$ is the number of transpositions required to turn $q_{i_1}\cdots q_{i_n}$ into $Q_1\cdots Q_k$.

Proof: See Prop A.1.

Corollary 1.1. ***Moments and cumulants in terms of $\boldsymbol{\Psi}$ expectation values.*** *In terms of expectation values, the moments and cumulants of a set $\{q_i\}$ of particle-hole operators can be expressed as*

$$\gamma(q_{i_1}\cdots q_{i_n}) \equiv \left.\frac{\partial^n M(\boldsymbol{\alpha})}{\partial\alpha_{i_n}\cdots\partial\alpha_{i_1}}\right|_{\boldsymbol{\alpha}=0} = \langle\Psi|\mathbf{:}q_{i_1}\cdots q_{i_n}\mathbf{:}|\Psi\rangle \tag{1.16}$$

$$\lambda(q_{i_1}\cdots q_{i_n}) \equiv \left.\frac{\partial^n K(\boldsymbol{\alpha})}{\partial\alpha_{i_n}\cdots\partial\alpha_{i_1}}\right|_{\boldsymbol{\alpha}=0} = \sum_{k=1}^{n}(-)^{k+1}(k-1)!\sum_{(Q_1\cdots Q_k)}^{\mathcal{P}_k(q_{i_1}\cdots q_{i_n})}(-)^{n_{\mathbf{Q}}}\langle\Psi|\mathbf{:}Q_1\mathbf{:}|\Psi\rangle\cdots\langle\Psi|\mathbf{:}Q_k\mathbf{:}|\Psi\rangle \tag{1.17}$$

which follows directly from equations 1.10 and 1.15.

Corollary 1.2. ***The first non-vanishing moments equal their cumulants.*** *If all moments of fewer than n operators vanish then*

$$\lambda(q_{i_1}\cdots q_{i_n}) = \gamma(q_{i_1}\cdots q_{i_n}) \tag{1.18}$$

for all $q_{i_1},\ldots,q_{i_n}$, which follows from equation 1.15.

2 Ψ-normal ordering

Definition 2.1. ***Generalized contractions.*** *Generalized contractions* are of a set of particle-hole operators $\{q_i\}$ are a set of scalar functions of one or more of these operators

$$\{\overline{q}_{i_1},\ \overline{q_{i_1}q_{i_2}},\ \overline{q_{i_1}q_{i_2}q_{i_3}},\ \overline{q_{i_1}q_{i_2}q_{i_3}q_{i_4}},\ldots\}$$

i.e. each n-tuple contraction $\overline{q_{i_1}q_{i_2}\cdots q_{i_n}}$ associates a scalar value with the ordered list of operators $(q_{i_1},q_{i_2},\ldots,q_{i_n})$.

Definition 2.2. ***$\boldsymbol{\Psi}$-normal order and $\boldsymbol{\Psi}$-normal contractions.*** The Ψ-*normal order* for particle-hole operator strings $q_1\cdots q_n$ is defined as[2]

$$\vdots q_1\cdots q_n\vdots \equiv q_1\cdots q_n - \mathbf{:}\overline{q_1\cdots q_n}\mathbf{:}$$

where the generalized contractions are chosen such that $\langle\Psi|\vdots q_1\cdots q_n\vdots|\Psi\rangle = 0$ for all n. The sets of generalized contractions satisfying these conditions are called Ψ-*normal contractions*. Note that this "ordering" is defined such that Ψ behaves like vac does under vac-normal ordering. In particular, **??** carries over for the new normal ordering as $\langle\Psi|Q|\Psi\rangle = \overline{\overline{Q}}$, where the sum of complete contractions $\overline{\overline{Q}}$ now involves more than pairwise contractions.

[2] $\mathbf{:}\overline{q_1\cdots q_n}\mathbf{:}$ is defined by analogy with **??**, i.e. the sum of all possible combinations of generalized contractions

Proposition 2.1. ***Odd contractions vanish.*** *For odd n, $\overbracket{q_{i_1} q_{i_2} \cdots q_{i_n}} = 0$ if this is a Ψ-normal contraction and Ψ has a fixed particle number.*

Proof: Applying **??** to a single particle-hole operator, we have $\overline{q} = \langle\Psi|q|\Psi\rangle = 0$ since Ψ has a definite particle number.[3] Now, assume the conclusion holds for odd n and consider the $(n+2)$-tuple contraction $\overbracket{q_{i_1} q_{i_2} \cdots q_{i_{n+2}}}$. By **??** we have $\langle\Psi|q_{i_1}\cdots q_{i_{n+2}}|\Psi\rangle = \overline{\overline{q_{i_1}\cdots q_{i_{n+2}}}}\,' + \overbracket{q_{i_1} q_{i_2} \cdots q_{i_{n+2}}}$ where the prime indicates that the $(n+2)$-tuple contraction has been separated out. Since Ψ has a definite particle number, we have $\langle\Psi|q_{i_1}\cdots q_{i_{n+2}}|\Psi\rangle = 0$. Furthermore, every term in $\overline{\overline{q_{i_1}\cdots q_{i_{n+2}}}}\,'$ must involve an odd contraction of order n or less in order to fully contract the product, which means that this term vanishes as well. This leaves $\overbracket{q_{i_1} q_{i_2} \cdots q_{i_{n+2}}} = 0$, so the conclusion holds in general.

2.1 Generalized Wick's theorem

Lemma 2.1. *The Ψ expectation value of a string Q of particle-hole operators is given by*

$$\langle\Psi|Q|\Psi\rangle = \sum_{(Q_1\cdots Q_k)}^{\mathcal{P}(Q)} (-)^{n_{\mathbf{Q}}}\ \overbracket{Q}_1 \cdots \overbracket{Q}_k \tag{2.1}$$

where $\overbracket{Q}$ represents $\overbracket{q_{i_1} q_{i_2} \cdots q_{i_n}}$, a contraction of all of the operators in Q, and $\mathcal{P}(Q)$ are product partitions of Q. $n_{\mathbf{Q}}$ is the number of transpositions required to achieve the permutation $Q \mapsto Q_1 \cdots Q_k$.

Proof: By **??**, we have $\langle\Psi|Q|\Psi\rangle = \overline{\overline{Q}}$. Furthermore, each complete contraction of Q partitions of its operators into disjoint subsets $(Q_1, \ldots, Q_k)$ of operators that are contracted with each other. Finally, disentangling the contracted product is achieved by a permutation which places contraction partners adjacent to each other, i.e. $Q \mapsto Q_1 \cdots Q_k$. The signature of such a permutation, $(-)^{n_{\mathbf{Q}}}$, is unambiguous because odd contractions vanish (see Prop 2.1). Therefore, $\langle\Psi|Q|\Psi\rangle = \overline{\overline{Q}} = \sum_{\mathbf{Q}}^{\mathcal{P}(Q)} (-)^{n_{\mathbf{Q}}}\ \overbracket{Q}_1 \cdots \overbracket{Q}_k$.

Theorem 2.1. ***Generalized Wick's theorem.*** *Any operator Q which is in* vac*-normal order ($\vdots\vdots$) can be expanded as*

$$Q = \vdots Q \vdots + \vdots \overline{Q} \vdots \tag{2.2}$$

where $\vdots\vdots$ inticates a Ψ-normal-ordered product and the generalized Ψ-normal contractions are cumulants. That is,

$$\overbracket{q_{i_1} q_{i_2} \cdots q_{i_n}} = \lambda(q_{i_1} \cdots q_{i_n}) \tag{2.3}$$

for each n-tuple contraction in $\vdots \overline{Q} \vdots$.

Proof: Equation 2.2 is required by Def 2.2, so it remains to be proven that the Ψ-normal contractions are cumulants. The theorem holds for $n = 2$ since $\langle\Psi|q_{i_1} q_{i_2}|\Psi\rangle = \overbracket{q_{i_1} q_{i_2}}$ follows from Lem 2.1 and $\langle\Psi|q_{i_1} q_{i_2}|\Psi\rangle = \gamma(q_{i_1} q_{i_2}) = \lambda(q_{i_1} q_{i_2})$ by Cor 1.2. Now, assume it holds for all contractions up to n and consider $\overbracket{Q}$ for Q of length n. By Lem 2.1, we have

$$\langle\Psi|Q|\Psi\rangle = \gamma(Q) = \overbracket{Q} + \sum_{k=1}^{n-1} \sum_{(Q_1\cdots Q_k)}^{\mathcal{P}_k(Q)} (-)^{n_{\mathbf{Q}}}\ \overbracket{Q}_1 \cdots \overbracket{Q}_k$$

which gives

$$\overbracket{Q} = \gamma(Q) - \sum_{k=1}^{n-1} \sum_{(Q_1\cdots Q_k)}^{\mathcal{P}_k(Q)} (-)^{n_{\mathbf{Q}}}\ \lambda(Q_1) \cdots \lambda(Q_k)$$

which implies $\overbracket{Q} = \lambda(Q)$ from the moment-cumulant relations (Prop 1.2, equation 1.14). By induction, the claim holds for all n.

[3] Each $\mathbb{A}(\mathcal{H}^{\otimes n}) \subset F(\mathcal{H})$ forms an orthogonal subspace of $F(\mathcal{H})$.

A Derivation of the moment-cumulant relations

Note: In this section, sums $\sum_n$ and $\sum_k$ without specified ranges should be taken to run from 1 to ∞.

Proposition A.1. ***Moment-cumulant relations (general).*** *The moments and cumulants of a set $\{q_i\}$ of random variables are related via*

$$\gamma(q_{i_1}\cdots q_{i_n}) = \sum_{k=1}^{n} \sum_{(Q_1\cdots Q_k)}^{\mathcal{P}_k(q_{i_1}\cdots q_{i_n})} (-)^{m\cdot n_{\mathbf{Q}}} \lambda(Q_1)\cdots\lambda(Q_k) \tag{A.1}$$

$$\lambda(q_{i_1}\cdots q_{i_n}) = \sum_{k=1}^{n} (-)^{k+1}(k-1)! \sum_{(Q_1\cdots Q_k)}^{\mathcal{P}_k(q_{i_1}\cdots q_{i_n})} (-)^{m\cdot n_{\mathbf{Q}}} \gamma(Q_1)\cdots\gamma(Q_k) \tag{A.2}$$

where $m = 0$ for commuting random variables and $m = 1$ for particle-hole operators.

Proof: The generating functions are

$$M(\boldsymbol{\alpha}) = \exp K(\boldsymbol{\alpha}) = 1 + \sum_n \sum_{i_1\cdots i_n} \frac{\alpha_{i_1}\cdots\alpha_{i_n}}{n!}\gamma(q_{i_1}\cdots q_{i_n})$$

$$K(\boldsymbol{\alpha}) = \ln M(\boldsymbol{\alpha}) = 0 + \sum_n \sum_{i_1\cdots i_n} \frac{\alpha_{i_1}\cdots\alpha_{i_n}}{n!}\lambda(q_{i_1}\cdots q_{i_n})$$

where $\{\alpha_i\}$ are either ordinary numbers or Grassmann numbers. Defining $b_n \equiv \sum_{i_1\cdots i_n} \frac{\alpha_{i_1}\cdots\alpha_{i_n}}{n!}\gamma(q_{i_1}\cdots q_{i_n})$ and $c_n \equiv \sum_{i_1\cdots i_n} \frac{\alpha_{i_1}\cdots\alpha_{i_n}}{n!}\lambda(q_{i_1}\cdots q_{i_n})$, and Taylor expansion coefficients $T_k^{\exp} = \frac{1}{k!}$ and $T_k^{\ln} = \frac{(-)^{k+1}}{k}$, these can be expanded as

$$M(\boldsymbol{\alpha}) = \exp(0 + \sum_n c_n) = 1 + \sum_k T_k^{\exp} \sum_{n_1\cdots n_k} c_{n_1}\cdots c_{n_k}$$

$$K(\boldsymbol{\alpha}) = \ln(1 + \sum_n b_n) = 0 + \sum_k T_k^{\ln} \sum_{n_1\cdots n_k} b_{n_1}\cdots b_{n_k}\ .$$

To group terms in the summation in powers of the α_i, the summations can be re-ordered using

$$\sum_k \sum_{n_1\cdots n_k} \alpha^{n_1+\cdots+n_k} f_{n_1}\cdots f_{n_k} = \sum_n \sum_{k=1}^{n} \sum_{(n_1\cdots n_k)}^{\mathcal{C}_k(n)} \alpha^n f_{n_1}\cdots f_{n_k} = \sum_n \sum_{k=1}^{n} k! \sum_{(n_1\cdots n_k)}^{\mathcal{P}_k(n)} \alpha^n f_{n_1}\cdots f_{n_k}$$

where $\mathcal{C}_k(n)$ and $\mathcal{P}_k(n)$ are k-tuple integer compositions and partitions (respectively) of n. That is, each $(n_1\cdots n_k)$ is a tuple of positive integers less than n such that $\sum_{i=1}^{k} n_i = n$. $\mathcal{C}_k(n)$ counts different orderings separately.[4] This rearrangement gives

$$M(\boldsymbol{\alpha}) = 1 + \sum_n \sum_{k=1}^{n} k! T_k^{\exp} \sum_{(n_1\cdots n_k)}^{\mathcal{P}_k(n)} c_{n_1}\cdots c_{n_k}$$

$$K(\boldsymbol{\alpha}) = 0 + \sum_n \sum_{k=1}^{n} k! T_k^{\ln} \sum_{(n_1\cdots n_k)}^{\mathcal{P}_k(n)} b_{n_1}\cdots b_{n_k}$$

and expanding each b_{n_i} and c_{n_i} produces

$$M(\boldsymbol{\alpha}) = 1 + \sum_n \sum_{i_1\cdots i_n} \alpha_{i_1}\cdots\alpha_{i_n} \sum_{k=1}^{n} k! T_k^{\exp} \sum_{(n_1\cdots n_k)}^{\mathcal{P}_k(n)} \frac{1}{n_1!\cdots n_k!}\lambda(q_{i_1}\cdots q_{i_{n_1}})\cdots\lambda(q_{i_{n-n_k+1}}\cdots q_{i_n})$$

$$K(\boldsymbol{\alpha}) = 0 + \sum_n \sum_{i_1\cdots i_n} \alpha_{i_1}\cdots\alpha_{i_n} \sum_{k=1}^{n} k! T_k^{\ln} \sum_{(n_1\cdots n_k)}^{\mathcal{P}_k(n)} \frac{1}{n_1!\cdots n_k!}\gamma(q_{i_1}\cdots q_{i_{n_1}})\cdots\gamma(q_{i_{n-n_k+1}}\cdots q_{i_n})\ .$$

[4]Example: the *partitions* of 3 are $\mathcal{P}(3) = \{(3), (2\ 1), (1\ 1\ 1)\}$ and its *compositions* are $\mathcal{C}(3) = \{(3), (2\ 1), (1\ 2), (1\ 1\ 1)\}$. The *2-tuple partitions* of 3 are $\mathcal{P}_2(3) = \{(2\ 1)\}$ and its *2-tuple compositions* are $\mathcal{C}_2(3) = \{(2\ 1), (1\ 2)\}$.

Taking derivatives with respect to the generator arguments, we find

$$\left.\frac{\partial^n M(\boldsymbol{\alpha})}{\partial\alpha_{i_n}\cdots\partial\alpha_{i_1}}\right|_{\boldsymbol{\alpha}=0} = \sum_{k=1}^{n} k!T_k^{\exp} \sum_{(n_1\cdots n_k)}^{\mathcal{P}_k(n)} \frac{1}{n_1!\cdots n_k!} \sum_{\pi}^{\mathrm{S}_n} \varepsilon_\pi^m \lambda(q_{i_{\pi(1)}}\cdots q_{i_{\pi(n_1)}})\cdots\lambda(q_{i_{\pi(n-n_k+1)}}\cdots q_{i_{\pi(n)}})$$

$$\left.\frac{\partial^n K(\boldsymbol{\alpha})}{\partial\alpha_{i_n}\cdots\partial\alpha_{i_1}}\right|_{\boldsymbol{\alpha}=0} = \sum_{k=1}^{n} k!T_k^{\ln} \sum_{(n_1\cdots n_k)}^{\mathcal{P}_k(n)} \frac{1}{n_1!\cdots n_k!} \sum_{\pi}^{\mathrm{S}_n} \varepsilon_\pi^m \gamma(q_{i_{\pi(1)}}\cdots q_{i_{\pi(n_1)}})\cdots\gamma(q_{i_{\pi(n-n_k+1)}}\cdots q_{i_{\pi(n)}})$$

where $m = 0$ when the α_i are ordinary variables and $m = 1$ when they are Grassmann variables. The summations over integer partitions can be re-written in terms of product partitions of $q_{i_1}\cdots q_{i_n}$, defined by analogy with set partitions.

$$\sum_{(n_1\cdots n_k)}^{\mathcal{P}_k(n)} \frac{1}{n_1!\cdots n_k!} \sum_{\pi}^{\mathrm{S}_n} \varepsilon_\pi^m f(q_{i_{\pi(1)}}\cdots q_{i_{\pi(n_1)}})\cdots f(q_{i_{\pi(n-n_k+1)}}\cdots q_{i_{\pi(n)}}) = \sum_{(Q_1\cdots Q_k)}^{\mathcal{P}_k(q_{i_1}\cdots q_{i_n})} (-)^{m\cdot n_{\mathbf{Q}}} f(Q_1)\cdots f(Q_k)$$

This comes from the fact that for each product $f(q_{i_{\pi(1)}}\cdots q_{i_{\pi(n_1)}})\cdots f(q_{i_{\pi(n-n_k+1)}}\cdots q_{i_{\pi(n)}})$ there are exactly $n_1!\cdots n_k!$ permutations of the operators within each argument, and these terms are equal (up to a phase factor). These symmetries of γ and λ come from the fact that $\frac{\partial^n}{\partial\alpha_1\cdots\partial\alpha_n} = \varepsilon_\pi^m \frac{\partial^n}{\partial\alpha_{\pi(1)}\cdots\partial\alpha_{\pi(n)}}$ for all $\pi \in \mathrm{S}_n$. This rearrangement leaves

$$\left.\frac{\partial^n M(\boldsymbol{\alpha})}{\partial\alpha_{i_n}\cdots\partial\alpha_{i_1}}\right|_{\boldsymbol{\alpha}=0} = \sum_{k=1}^{n} k!T_k^{\exp} \sum_{(Q_1\cdots Q_k)}^{\mathcal{P}_k(q_{i_1}\cdots q_{i_n})} (-)^{m\cdot n_{\mathbf{Q}}} \lambda(Q_1)\cdots\lambda(Q_k)$$

$$\left.\frac{\partial^n K(\boldsymbol{\alpha})}{\partial\alpha_{i_n}\cdots\partial\alpha_{i_1}}\right|_{\boldsymbol{\alpha}=0} = \sum_{k=1}^{n} k!T_k^{\ln} \sum_{(Q_1\cdots Q_k)}^{\mathcal{P}_k(q_{i_1}\cdots q_{i_n})} (-)^{m\cdot n_{\mathbf{Q}}} \gamma(Q_1)\cdots\gamma(Q_k)$$

which, on plugging in $k!T_k^{\ln} = (-)^{k+1}(k-1)!$ and $k!T_k^{\exp} = 1$, gives the final result:

$$\gamma(q_{i_1}\cdots q_{i_n}) \equiv \left.\frac{\partial^n M(\boldsymbol{\alpha})}{\partial\alpha_{i_n}\cdots\partial\alpha_{i_1}}\right|_{\boldsymbol{\alpha}=0} = \sum_{k=1}^{n} \sum_{(Q_1\cdots Q_k)}^{\mathcal{P}_k(q_{i_1}\cdots q_{i_n})} (-)^{m\cdot n_{\mathbf{Q}}} \lambda(Q_1)\cdots\lambda(Q_k)$$

$$\lambda(q_{i_1}\cdots q_{i_n}) \equiv \left.\frac{\partial^n K(\boldsymbol{\alpha})}{\partial\alpha_{i_n}\cdots\partial\alpha_{i_1}}\right|_{\boldsymbol{\alpha}=0} = \sum_{k=1}^{n} (-)^{k+1}(k-1)! \sum_{(Q_1\cdots Q_k)}^{\mathcal{P}_k(q_{i_1}\cdots q_{i_n})} (-)^{m\cdot n_{\mathbf{Q}}} \gamma(Q_1)\cdots\gamma(Q_k)\ .$$