General Wick's theorem for bosonic and fermionic operators

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Wick's theorem provides a connection between time ordered products of bosonic or fermionic fields, and their normal ordered counterparts. We consider a generic pair of operator orderings and we prove, by induction, the theorem that relates them. We name this the general Wick's theorem (GWT) because it carries Wick's theorem as special instance, when one applies the GWT to time and normal orderings. We establish the GWT both for bosonic and fermionic operators, i.e., operators that satisfy c-number commutation and anticommutation relations respectively. We remarkably show that the GWT is the same, independent of the type of operator involved. By means of a few examples, we show how the GWT helps treat demanding problems by reducing the amount of calculations required.

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I. INTRODUCTION

Ever since the advent of quantum mechanics, various rules of operator orderings have been considered, e.g., in canonical quantization [1], phase space representation [2], field theory [3–7], quantum optics [8], and statistical physics [9]. Time ordering $\mathcal{T}$ and normal ordering $\mathcal{N}$ of quantized fields $\hat{\phi}(x)$ are paradigmatic in relativistic quantum field theory. These orderings are related by Wick's theorem [5], whose conception proved crucial essentially in any area of theoretical physics, because it allows for calculating the matrix elements of the (time-ordered) evolution operator. Wick's theorem for exponential test functionals of a free bosonic or fermionic field $\hat{\phi}(x)$ can be written into the compact form [10],

$$\mathcal{T}[e^{\int\lambda(x)\hat{\phi}(x)d^4x}] = e^C\mathcal{N}[e^{\int\lambda(x)\hat{\phi}(x)d^4x}], \tag{1}$$

where $\lambda(x)$ is an arbitrary c-number field and C is its quadratic functional

$$C = \frac{1}{2}\iint C(x,y)\lambda(x)\lambda(y)d^4xd^4y\,, \tag{2}$$

where $C(x,y)$ is the kernel of *Wick's contraction*:

$$C(x,y) = \mathcal{T}\hat{\phi}(x)\hat{\phi}(y) - \mathcal{N}\hat{\phi}(x)\hat{\phi}(y) \equiv (\mathcal{T}-\mathcal{N})\hat{\phi}(x)\hat{\phi}(y). \tag{3}$$

Two further forms [6,7] of Wick's original theorem were proven for arbitrary functionals $\mathcal{F}$ instead of the exponential test functionals in Eq. (1):

$$\mathcal{T}[\mathcal{F}(\hat{\phi})] = \mathcal{N}[\mathcal{F}(\hat{\phi}')], \tag{4}$$

$$\mathcal{T}[\mathcal{F}(\hat{\phi})] = e^\Gamma\mathcal{N}[\mathcal{F}(\hat{\phi})], \tag{5}$$

where $\hat{\phi}'(x) = \hat{\phi}(x) + \int C(x,y)\frac{\delta}{\delta\phi(y)}d^4y$, and Γ is the quadratic form of the functional derivatives:

$$\Gamma = \frac{1}{2}\iint C(x,y)\frac{\delta}{\delta\phi(x)}\frac{\delta}{\delta\phi(y)}d^4xd^4y\,. \tag{6}$$

Wick's seminal work was extended in different ways, so the literature of "generalized Wick's theorem" includes very different kinds of generalizations, such as spin chains [11,12], generalized normal order in quantum chemistry [13,14], thermal field theory [15–17], phase-space representation of time ordering against a generic ordering [18,19], nonequilibrium Green's functions [20], and multiphonon theory [21].

We follow the direction first taken in Ref. [22], where it was suggested that the theorem in Eqs. (1)–(3) still holds if $\mathcal{T}$ and $\mathcal{N}$ are replaced by any pair $\mathcal{O}$, $\mathcal{O}'$ of generic orderings. With these replacements, Eq. (1) is called the *general Wick's theorem* (GWT), while Eq. (3) defines the general contraction. A tentative proof of GWT for bosonic operators was provided in Ref. [22], which was circumstantial but gave a strong indication of its correctness.

In this paper, not only do we confirm the correctness of the intuition in Ref. [22] for GWT with bosonic operators, but also our major result is the unique form of GWT for the pair of generic orderings for bosonic and fermionic operators together. Precisely, we consider the forms (4) and (5) of Wick's theorem, and we prove the ultimate form of GWT:

$$\begin{aligned}\mathcal{O}[\mathcal{F}(\hat{\phi})] &= e^\Gamma\mathcal{O}'[\mathcal{F}(\hat{\phi})],\\ C(x,y) &= (\mathcal{O}-\mathcal{O}')\hat{\phi}(x)\hat{\phi}(y),\end{aligned} \tag{7}$$

valid no matter if $\hat{\phi}$'s are bosonic or fermionic or both together.

The paper is organized as follows: In Secs. II and III we respectively introduce the definitions of operator orderings

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and contractions. In Sec. IV we prove the GWT for bosonic operators by induction, while in Sec. V we outline the proof for fermionic operators. In Sec. VI we provide two applications of the GWT, namely to the Baker-Campbell-Hausdorff formula and to quadratic forms, and in Sec. VII we draw our conclusions.

II. OPERATOR ORDERINGS

We consider a set of operators $\hat{\phi}_\alpha$ with α belonging to some ordered index set Ω. An ordering operator $\mathcal{O}$ rearranges the elements of an input product of operators, to output a suitably ordered one. Orderings $\mathcal{O}$ can be bosonic or fermionic, defined by

$$\mathcal{O}[\hat{\phi}_1 \dots \hat{\phi}_n] = (\pm 1)^P \hat{\phi}_{p_1} \dots \hat{\phi}_{p_n}, \tag{8}$$

when for simplicity's sake the index set Ω consists of integers. Here P is the number of permutations that bring the initial string of indexes $1 \dots n$ to the ordered one $p_1 \succ p_2 \succ \dots \succ p_n$. The signature ± 1 distinguishes bosonic orderings $(+1)$ from fermionic ones (-1). Accordingly, fermionic orderings are sensitive to the order of the operators in the input string, but bosonic orderings are not. By bosonic and/or fermionic operators, we mean any set of operators satisfying c-number commutation and/or anticommutation relations: $[\hat{\phi}_\alpha, \hat{\phi}_\beta]_\pm \in \mathbb{C}$ (where $[\cdot,\cdot]_- = [\cdot,\cdot]$ and $[\cdot,\cdot]_+ = \{\cdot,\cdot\}$). The identity (8) can be trivially extended to composite indices, the paradigmatic example being the time ordering of fields $\hat{\phi}(x) = \hat{\phi}(t, \boldsymbol{x})$. We take the occasion to clarify an issue that is often overlooked. In our definition (8), we follow Wick, who observed that validity of his theorem required the introduction of the sign $(-1)^P$ for fermionic orderings $\mathcal{T}, \mathcal{N}$ [5]. So, Wick's time ordering of fermionic fields differ from Dysons's [4], which does not contain the sign $(-1)^P$. Accordingly, fermionic Wick's theorem in general cannot be applied to Dyson-ordered evolution operators for fermionic systems (see, e.g., Ref. [23]). In quantum electrodynamics, this constitutes no issue because the electromagnetic field couples to the current which is local quadratic in the fields: Dyson's and Wick's orderings coincide in this case.

When we talk about a different ordering $\mathcal{O}'$ of the same product $\hat{\phi}_1 \dots \hat{\phi}_n$, it may be a different permutation of the field operators, but it will be more general than that. We assume that the operators $\hat{\phi}_\alpha$ are linear combinations of operators $\hat{\varphi}_k$, with k possibly belonging to some different index set Ω',

$$\hat{\phi}_\alpha = \mathcal{L}_{\alpha k} \hat{\varphi}_k, \tag{9}$$

where and henceforth we assume the Einstein convention for repeated indexes, with the additional condition that sums always run on all the elements of the respective index sets. Here we assume that Ω and Ω' are discrete sets but the following analysis holds true invariably for continuous sets, provided that sums are replaced by integrals, functions become functionals, matrices become kernels, and partial derivatives are replaced by functional derivatives. We postulate that $\mathcal{O}'$ orders the products of the operators $\hat{\varphi}_k$. To be as general as possible, $\mathcal{O}$ orders (products of) $\hat{\phi}_\alpha$'s, cf. Eq. (8), but it does not order $\hat{\varphi}_k$'s. Similarly, $\mathcal{O}'$ orders $\hat{\varphi}_k$'s, but does not order $\hat{\phi}_\alpha$'s. A simple example to keep in mind is $\{\hat{\phi}\} = \hat{q}, \hat{p}$, $\mathcal{O} = qp$ ordering, $\{\hat{\varphi}\} = a, a^\dagger$, $\mathcal{O}' = \mathcal{N}$. Still, we define $\mathcal{O}'$ ordering of the $\hat{\phi}$'s indirectly, using the expansion (9):

$$\mathcal{O}'[\hat{\phi}_{\alpha_1} \dots \hat{\phi}_{\alpha_n}] \equiv \left(\prod_{i=1}^n \mathcal{L}_{\alpha_i k_i} \right) \mathcal{O}'[\hat{\varphi}_{k_1} \dots \hat{\varphi}_{k_n}]. \tag{10}$$

The assumption of the linear relationship (9) allows for a simpler and more transparent proof of GWT compared to the tentative proof in Ref. [22]. Then the result can shortly be extended for the case of the more generic, implicit linear relationship [cf. (14)].

III. CONTRACTIONS

Given the pair of orderings $\mathcal{O}, \mathcal{O}'$ interpreted in Sec. II, we define the matrix of their contraction:

$$\mathcal{C}_{\alpha\beta} = (\mathcal{O} - \mathcal{O}')\hat{\phi}_\alpha \hat{\phi}_\beta, \tag{11}$$

which is symmetric [antisymmetric] if the $\hat{\phi}_\alpha$'s are bosonic [fermionic], respectively. Using Eqs. (9) and (10), we can detail the right-hand side as follows:

$$\begin{aligned} \mathcal{C}_{\alpha\beta} &= \theta_{l \succ k} \mathcal{L}_{\alpha k} \mathcal{L}_{\beta l} [\hat{\varphi}_k, \hat{\varphi}_l]_\pm - \theta_{\beta \succ \alpha} [\hat{\phi}_\alpha, \hat{\phi}_\beta]_\pm \\ &= (\theta_{\alpha \succ \beta} - \theta_{k \succ l}) [\hat{\phi}_\alpha, \hat{\phi}_\beta]_\pm, \end{aligned} \tag{12}$$

where we introduced the step function: $\theta_{\beta \succ \alpha} = 1$ if $\beta \succ \alpha$ and zero if $\alpha \succ \beta$. About our compact notations in the second line, we stress that $\mathcal{O}'$ ordering of the operators $\hat{\phi}_\alpha$ and $\hat{\phi}_\beta$ refers to their expansion (9) in terms of the operators $\hat{\varphi}_k$ and $\hat{\varphi}_l$, respectively. When $\mathcal{O} = \mathcal{T}$ and $\mathcal{O}' = \mathcal{N}$ to order quantum fields $\hat{\phi}(x)$ the index set $\Omega = \{x\}$ becomes continuous, and our generalized contraction (11) yields Wick's contraction (3) as it should. Along our forthcoming derivations, we need the matrix $\tilde{\mathcal{C}}_{kl}$ of contraction in terms of the $\hat{\varphi}_k$'s:

$$\tilde{\mathcal{C}}_{kl} = (\mathcal{O} - \mathcal{O}')\hat{\varphi}_k \hat{\varphi}_l, \tag{13}$$

satisfying $\mathcal{L}_{\alpha k} \mathcal{L}_{\beta l} \tilde{\mathcal{C}}_{kl} = \mathcal{C}_{\alpha\beta}$.

Contractions exist also when the operators $\hat{\phi}_\alpha$ cannot be expressed by linear combinations of the $\hat{\varphi}_k$'s like in Eq. (9) but the following implicit linear relationship with some coefficients λ_α and $\tilde{\lambda}_k$ does exist for them (cf. Ref. [22]),

$$\lambda_\alpha \hat{\phi}_\alpha = \tilde{\lambda}_k \hat{\varphi}_k \, (\equiv \hat{X}), \tag{14}$$

where the last identity simply defines the operator $\hat{X}$. This is essentially a generalization of (9), retaining the minimal requirement of linear relationship between the $\mathcal{O}$-ordered $\hat{\phi}_\alpha$'s and the $\mathcal{O}'$-ordered $\hat{\varphi}_k$'s. A simple example to keep in mind is $\{\hat{\phi}\} = \{\hat{f}_1 + \hat{f}_2, \hat{f}_3\}$, $\{\hat{\varphi}\} = \{\hat{f}_1, \hat{f}_2 + \hat{f}_3\}$; a relation of the type (9) cannot be established between $\hat{\phi}$ and $\hat{\varphi}$, but (14) holds. The contraction between $\mathcal{O}$ and $\mathcal{O}'$ can now be established in two steps. First, we consider the contraction between the trivial "ordering" of the lonely operator $\hat{X}$ and the $\mathcal{O}$ ordering of the $\hat{\phi}_\alpha$'s. Note that that $\hat{X} = \lambda_\alpha \hat{\phi}_\alpha$, which corresponds to Eq. (9), so the previously defined contraction (11) applies, and it applies similarly between the trivial ordering of $\hat{X}$ and the $\mathcal{O}'$ ordering of the $\hat{\varphi}_k$'s:

$$\mathcal{C}^{X\phi} = \hat{X}^2 - \mathcal{O}\hat{X}^2, \tag{15}$$

$$\mathcal{C}^{X\varphi} = \hat{X}^2 - \mathcal{O}'\hat{X}^2. \tag{16}$$

Second, we obtain the contraction between $\mathcal{O}$ and $\mathcal{O}'$:

$$\mathcal{C} = \mathcal{C}^{X\varphi} - \mathcal{C}^{X\phi} = (\mathcal{O} - \mathcal{O}')\hat{X}^2 = \mathcal{C}_{\alpha\beta}\lambda_\alpha\lambda_\beta. \tag{17}$$

In the special case when the explicit relationship (9) holds, the above equation determines the matrix $\mathcal{C}_{\alpha\beta}$ uniquely and in accordance with (11); otherwise we shall rely on the scalar contraction $\mathcal{C}$.

IV. BOSONIC GWT

We aim at proving that the $\mathcal{O}$ ordering of any function F of operators $\hat{\phi}_\alpha$, with shorthand notation $F(\hat{\phi})$, can be rewritten as the $\mathcal{O}'$ ordering of the same function of new operators $\hat{\phi}'_\alpha$, namely

$$\mathcal{O}[F(\hat{\phi})] = \mathcal{O}'[F(\hat{\phi}')]\,, \tag{18}$$

with

$$\hat{\phi}'_\alpha \equiv \hat{\phi}_\alpha + \mathcal{C}_{\alpha\beta}\partial_\beta\,, \tag{19}$$

$\mathcal{C}_{\alpha\beta}$ is the matrix of contraction (11), and $\partial_\beta = \partial/\partial\phi_\beta$ is a standard c-number derivative (see the Appendix for further details on the specific meaning of such derivatives). On the right-hand side of GWT (18) it is to be understood that before the $\mathcal{O}'$ ordering we express the operators $\hat{\phi}'_\alpha$ in terms of the operators $\hat{\varphi}'_k$; cf. (10). Exploiting (9), we can write

$$\hat{\phi}'_\alpha = \mathcal{L}_{\alpha k}\hat{\varphi}'_k, \tag{20}$$

$$\hat{\varphi}'_k = \hat{\varphi}_k + \tilde{\mathcal{C}}_{kl}\tilde{\partial}_l, \tag{21}$$

with notation $\tilde{\partial}_l = \partial/\partial\varphi_l$, and where we recall that the matrix $\tilde{\mathcal{C}}_{kl}$ satisfies $\mathcal{L}_{\alpha k}\mathcal{L}_{\beta l}\tilde{\mathcal{C}}_{kl} = \mathcal{C}_{\alpha\beta}$. Since any operator functional can be expanded in power series, we will work with products of operators. We prove the GWT by induction: We assume that

$$\mathcal{O}\left[\prod_{i=1}^{n}\hat{\phi}_{\alpha_i}\right] = \mathcal{O}'\left[\prod_{i=1}^{n}\hat{\phi}'_{\alpha_i}\right] \tag{22}$$

holds up to a given n (the cases $n = 0$ and $n = 1$ are trivially true), and we prove that

$$\mathcal{O}\left[\hat{\phi}_\alpha\prod_{i=1}^{n}\hat{\phi}_{\alpha_i}\right] = \mathcal{O}'\left[\hat{\phi}'_\alpha\prod_{i=1}^{n}\hat{\phi}'_{\alpha_i}\right]. \tag{23}$$

Let us assume that $\mathcal{O}$ orders the operators $\hat{\phi}$ with decreasing index from left to right, i.e., $\alpha_n \succ \cdots \succ \alpha_1$:

$$\mathcal{O}\left[\prod_{i=1}^{n}\hat{\phi}_{\alpha_i}\right] = \hat{\phi}_{\alpha_n}\ldots\hat{\phi}_{\alpha_1}\,, \tag{24}$$

We can thus rewrite the left-hand side of Eq. (23) as follows:

$$\mathcal{O}\left[\hat{\phi}_\alpha\prod_{i=1}^{n}\hat{\phi}_{\alpha_i}\right] = \hat{\phi}_{\alpha_n}\ldots\hat{\phi}_{\alpha_{j+1}}\hat{\phi}_\alpha\hat{\phi}_{\alpha_j}\ldots\hat{\phi}_{\alpha_1}\,, \tag{25}$$

where $\alpha_n \succ \cdots \succ \alpha_{j+1} \succ \alpha \succ \alpha_j \succ \cdots \succ \alpha_1$. In order to be able to exploit Eq. (22), we need to bring $\hat{\phi}_\alpha$ outside the product, and we arbitrarily choose to do so by moving $\hat{\phi}_\alpha$ to the left (needless to say, the GWT can be equivalently proved also by moving $\hat{\phi}_\alpha$ to the right). This can be done by exploiting the following identity:

$$\hat{\phi}_{\alpha_n}\ldots\hat{\phi}_{\alpha_{j+1}}\hat{\phi}_\alpha\hat{\phi}_{\alpha_j}\ldots\hat{\phi}_{\alpha_1} = \hat{\phi}_{\alpha_n}\ldots\hat{\phi}_\alpha\hat{\phi}_{\alpha_{j+1}}\hat{\phi}_{\alpha_j}\ldots\hat{\phi}_{\alpha_1} - [\hat{\phi}_\alpha,\hat{\phi}_{\alpha_{j+1}}]\partial_{\alpha_j+1}\mathcal{O}\left[\prod_{i=1}^{n}\hat{\phi}_{\alpha_i}\right], \tag{26}$$

where α_{j+1} is the label of α's left neighbor, and Einstein summation does not apply to it. When iterated, this identity leads to

$$\mathcal{O}\left[\hat{\phi}_\alpha\prod_{i=1}^{n}\hat{\phi}_{\alpha_i}\right] = \hat{\phi}_\alpha\,\mathcal{O}\left[\prod_{i=1}^{n}\hat{\phi}_{\alpha_i}\right] - \theta_{\beta\succ\alpha}[\hat{\phi}_\alpha,\hat{\phi}_\beta]\partial_\beta\,\mathcal{O}\left[\prod_{i=1}^{n}\hat{\phi}_{\alpha_i}\right], \tag{27}$$

where the Einstein convention is reactivated.

We apply Eq. (22), i.e., GWT up to order n, yielding

$$\mathcal{O}\left[\hat{\phi}_\alpha\prod_{i=1}^{n}\hat{\phi}_{\alpha_i}\right] = \hat{\phi}'_\alpha\,\mathcal{O}'\left[\prod_{i=1}^{n}\hat{\phi}'_{\alpha_i}\right] - \mathcal{C}_{\alpha\beta}\partial_\beta\mathcal{O}'\left[\prod_{i=1}^{n}\hat{\phi}'_{\alpha_i}\right] - \theta_{\beta\succ\alpha}[\hat{\phi}_\alpha,\hat{\phi}_\beta]\partial_\beta\,\mathcal{O}'\left[\prod_{i=1}^{n}\hat{\phi}'_{\alpha_i}\right], \tag{28}$$

where we inserted $\hat{\phi}_\alpha = \hat{\phi}'_\alpha - \mathcal{C}_{\alpha\beta}\partial_\beta$. Let us concentrate on the first term on the right-hand side, onto which we exploit Eq. (20) in order to prepare for $\mathcal{O}'$ ordering:

$$\hat{\phi}'_\alpha\,\mathcal{O}'\left[\prod_{i=1}^{n}\hat{\phi}'_{\alpha_i}\right] = \mathcal{L}_{\alpha k}\left[\prod_{i=1}^{n}\mathcal{L}_{\alpha_i k_i}\right]\hat{\varphi}'_k\mathcal{O}'\left[\prod_{i=1}^{n}\hat{\varphi}'_{k_i}\right]. \tag{29}$$

The operator part on the right-hand side can further be written as

$$\hat{\varphi}'_k\mathcal{O}'\left[\prod_{i=1}^{n}\hat{\varphi}'_{k_i}\right] = \mathcal{O}'\left[\hat{\varphi}'_k\prod_{i=1}^{n}\hat{\varphi}'_{k_i}\right] + \theta_{l\succ k}[\hat{\varphi}'_k,\hat{\varphi}'_l]\tilde{\partial}_l\mathcal{O}'\left[\prod_{i=1}^{n}\hat{\varphi}'_{k_i}\right], \tag{30}$$

so that by reusing Eq. (20), Eq. (29) becomes

$$\hat{\phi}'_\alpha\,\mathcal{O}'\left[\prod_{i=1}^{n}\hat{\phi}'_{\alpha_i}\right] = \mathcal{O}'\left[\hat{\phi}'_\alpha\prod_{i=1}^{n}\hat{\phi}'_{\alpha_i}\right] + \mathcal{L}_{\alpha k}\theta_{l\succ k}[\hat{\varphi}'_k,\hat{\varphi}'_l]\tilde{\partial}_l\mathcal{O}'\left[\prod_{i=1}^{n}\hat{\phi}'_{\alpha_i}\right]. \tag{31}$$

With this, we can write Eq. (28) into this form:

$$\mathcal{O}\left[\hat{\phi}_\alpha\prod_{i=1}^{n}\hat{\phi}_{\alpha_i}\right] = \mathcal{O}'\left[\hat{\phi}'_\alpha\prod_{i=1}^{n}\hat{\phi}'_{\alpha_i}\right] + \mathcal{D}\mathcal{O}'\left[\prod_{i=1}^{n}\hat{\phi}'_{\alpha_i}\right], \tag{32}$$

where $\mathcal{D}$ is the following differential operator:

$$\mathcal{D} = \mathcal{L}_{\alpha k}\theta_{l\succ k}[\hat{\varphi}'_k,\hat{\varphi}'_l]\tilde{\partial}_l - \mathcal{C}_{\alpha\beta}\partial_\beta - \theta_{\beta\succ\alpha}[\hat{\phi}_\alpha,\hat{\phi}_\beta]\partial_\beta. \tag{33}$$

At this stage, we substitute the identity $\tilde{\partial}_l = \mathcal{L}_{\beta l}\partial_\beta$ and, invoking the definition (21), we can replace $[\hat{\varphi}'_k,\hat{\varphi}'_l] =$

$[\hat{\varphi}_k, \hat{\varphi}_l] + \tilde{\mathcal{C}}_{kl} - \tilde{\mathcal{C}}_{lk} = [\hat{\varphi}_k, \hat{\varphi}_l]$, yielding

$$\begin{aligned}\mathcal{D} &= [\mathcal{L}_{\alpha k}\mathcal{L}_{\beta l}\theta_{l\succ k}[\hat{\varphi}_k, \hat{\varphi}_l] - \theta_{\beta\succ\alpha}[\hat{\phi}_\alpha, \hat{\phi}_\beta] - \mathcal{C}_{\alpha\beta}]\partial_\beta \\ &= [(\theta_{\alpha\succ\beta} - \theta_{k\succ l})[\hat{\phi}_\alpha, \hat{\phi}_\beta] - \mathcal{C}_{\alpha\beta}]\partial_\beta\,. \end{aligned} \tag{34}$$

Induction is done and the GWT (18) is proven provided $\mathcal{D}$ vanishes, and this happens if we use the form (12) with commutator of the contraction $\mathcal{C}_{\alpha\beta}$. The GWT of (18) and (19) is thus proven.

Now we turn toward the proof of the ultimate form (7) of the GWT. There is a transformation of equivalence between each $\hat{\phi}'_\alpha$ and $\hat{\phi}_\alpha$:

$$\hat{\phi}'_\alpha = e^{\Gamma}\hat{\phi}_\alpha e^{-\Gamma}\,, \tag{35}$$

where

$$\Gamma = \tfrac{1}{2}\mathcal{C}_{\alpha\beta}\partial_\alpha\partial_\beta\,. \tag{36}$$

Equation (35) can be confirmed, e.g., by Taylor expanding the right-hand side:

$$\hat{\phi}_\alpha + [\Gamma, \hat{\phi}_\alpha] + \tfrac{1}{2}[\Gamma, [\Gamma, \hat{\phi}_\alpha]] + \cdots\,, \tag{37}$$

and observing that $[\Gamma, \hat{\phi}_\alpha] = \mathcal{C}_{\alpha\beta}\partial_\beta$, while higher order commutators are zero. This equivalence transformation allows us to write the GWT (18) in the following way:

$$\mathcal{O}[F(\hat{\phi})] = e^{\Gamma}\mathcal{O}'[F(\hat{\phi})]\,, \tag{38}$$

where $e^{-\Gamma}$ was dropped because the derivatives have nothing to act upon.

The above proofs of the two forms (18) and (38) of bosonic GWT required the explicit linear relationship (9). Here we are going to show that a similar GWT exists if (9) does not hold, but the weaker, implicit linear relationship (14) does. For this case, we defined the contraction $\mathcal{C} = (\mathcal{O} - \mathcal{O}')\hat{X}^2$ by Eq. (17). The GWT expresses $\mathcal{O}$ ordering of a function F in terms of $\mathcal{O}'$ ordering of F and therefore it must be possible to express F both in terms of $\hat{\phi}$ and of $\hat{\varphi}$. Accordingly, here we need to restrict the functions F to the class $F(\lambda_\alpha\hat{\phi}_\alpha) = F(\hat{X})$, that is an unavoidable compromise when (9) does not hold.

We are going to derive the form (38) of GWT between orderings $\mathcal{O}$ and $\mathcal{O}'$ in two steps, according to those in Sec. III. First, since $\hat{X}$ is a linear combination of the $\hat{\phi}_\alpha$'s, as well as of the $\hat{\varphi}_k$'s, we can apply GWT (38) between the trivial "ordering" of the lonely operator $\hat{X}$ and the $\mathcal{O}$ ordering of the $\hat{\phi}_\alpha$'s, and between $\hat{X}$ and the $\hat{\varphi}_k$'s as well:

$$\begin{aligned} F(\hat{X}) &= e^{\frac{1}{2}\mathcal{C}^{X\phi}\partial_X^2}\mathcal{O}[F(\hat{X})], \\ F(\hat{X}) &= e^{\frac{1}{2}\mathcal{C}^{X\varphi}\partial_X^2}\mathcal{O}'[F(\hat{X})]. \end{aligned} \tag{39}$$

Second, we get from here the GWT, extended from the case (9) to (14):

$$\mathcal{O}[F(\hat{X})] = e^{\frac{1}{2}\mathcal{C}\partial_X^2}\mathcal{O}'[F(\hat{X})]\,. \tag{40}$$

Note that invoking the second expression of $\mathcal{C}$ in (17) and using the chain rule of derivatives, we rewrite Eq.(40) as follows:

$$\mathcal{O}[F(\hat{X})] = e^{\frac{1}{2}\mathcal{C}_{\alpha\beta}\partial_\alpha\partial_\beta}\mathcal{O}'[F(\hat{X})], \tag{41}$$

which is the same form (36)–(38) that we derived for the direct relationship (9) except for the mentioned restriction on the form of the function F. We remark that if relation (14) holds for different sets (labeled by superscript i) $\{\lambda^i_\alpha\}$, then the GWT (41) holds for $F(\hat{X}^1, \hat{X}^2, \dots)$ with $\hat{X}^i = \lambda^i_\alpha\hat{\phi}_\alpha$. Eventually, if Eq. (14) holds for any choice of $\{\lambda^i_\alpha\}$, then (9) becomes existing and (41) yields Eq. (38), valid for $F(\hat{\phi})$ without restriction.

We add, for completeness, that on exponential test functions $F(\hat{X}) = e^{\hat{X}}$, our Eq. (41) yields

$$\mathcal{O}[e^{\hat{X}}] = e^{\frac{1}{2}\mathcal{C}_{\alpha\beta}\lambda_\alpha\lambda_\beta}\mathcal{O}'[e^{\hat{X}}] \tag{42}$$

which is the form of GWT proposed in Ref. [22] to generalize the form (1)–(3) of Wick's theorem.[1]

V. FERMIONIC GWT

The advantage of the functional approach is that it allows to extend the GWT to fermionic systems. Namely, we aim at proving the GWT [(18) and (19)], where now $\hat{\phi}$'s (and $\hat{\varphi}$'s) are fermionic operators (in the sense defined in Sec. II). We therefore retain the same setting as Secs. II–IV, in particular Eqs. (9), (12), (22), and (24), and we prove the GWT by induction. We recall that fermionic orderings depend on the initial order of the operators. In what follows, we nonetheless retain the simple notation $\prod_i\hat{\phi}_i$ for products of fermionic operators, which now denotes a definite initial ordering whose choice is arbitrary, and anyway cancels from the GWT. The equation corresponding to Eq. (25) for fermions reads

$$\mathcal{O}\left[\hat{\phi}_\alpha\prod_{i=1}^n\hat{\phi}_{\alpha_i}\right] = (-1)^{n-j}\hat{\phi}_{\alpha_n}\dots\hat{\phi}_{\alpha_{j+1}}\hat{\phi}_\alpha\hat{\phi}_{\alpha_j}\dots\hat{\phi}_{\alpha_1}\,, \tag{43}$$

where the factor $(-1)^{n-j}$ is due to the fact that the fermionic ordering brings a factor (-1) for each permutation. In order to move $\hat{\phi}_\alpha$ to the left we need to rewrite the right-hand side of this equation by iterating the following identity:

$$\begin{aligned} &\hat{\phi}_{\alpha_n}\dots\hat{\phi}_{\alpha_{j+1}}\hat{\phi}_\alpha\hat{\phi}_{\alpha_j}\dots\hat{\phi}_{\alpha_1} \\ &\quad= -\hat{\phi}_{\alpha_n}\dots\hat{\phi}_\alpha\hat{\phi}_{\alpha_{j+1}}\hat{\phi}_{\alpha_j}\dots\hat{\phi}_{\alpha_1} \\ &\qquad - (-1)^{n-j}\{\hat{\phi}_\alpha, \hat{\phi}_{\alpha_{j+1}}\}\partial_{\alpha_j+1}\mathcal{O}\left[\prod_{i=1}^n\hat{\phi}_{\alpha_i}\right], \end{aligned} \tag{44}$$

where the partial derivative is the standard Grassmann derivative, detailed in the Appendix. We can thus rewrite Eq. (43) as follows:

$$\begin{aligned}\mathcal{O}\left[\hat{\phi}_\alpha\prod_{i=1}^n\hat{\phi}_{\alpha_i}\right] &= \hat{\phi}_\alpha\,\mathcal{O}\left[\prod_{i=1}^n\hat{\phi}_{\alpha_i}\right] \\ &\quad - \theta_{\beta\succ\alpha}\{\hat{\phi}_\alpha, \hat{\phi}_\beta\}\partial_\beta\,\mathcal{O}\left[\prod_{i=1}^n\hat{\phi}_{\alpha_i}\right], \end{aligned} \tag{45}$$

which confirms that the initial ordering of operators is not influent for the proof of GWT. Remarkably, this equations has exactly the same structure as Eq. (27) for bosons. Accordingly, from here the proof of the fermionic GWT follows the lines of

[1] We take the opportunity to correct two typos in Ref. [22]. Expression (6) of contraction C should contain a factor 1/2 in front of the integral. The contraction (42) should read $C_t = (i\hbar/m)\int_0^t d\tau\int_0^\tau ds\,\tau F_\tau F_s$.

the bosonic one and we will not repeat it here. The final result is given by Eqs. (18) and (19) with the anticommutator form (12) for the contraction. We further remark that the form (38) of GWT holds also for fermions, with the same definition (36) for Γ.

An explicit form of GWT for fermionic fields $\hat{\psi}$ and $\hat{\psi}^\dagger$ can be easily obtained by considering the set $\{\hat{\phi}_\alpha\}_{\alpha=1}^{2n} = \{\hat{\psi}_1, \hat{\psi}_1^\dagger, \dots \hat{\psi}_n, \hat{\psi}_n^\dagger\}$. Since $\{\hat{\psi}_\alpha, \hat{\psi}_\beta\} = \{\hat{\psi}_\alpha^\dagger, \hat{\psi}_\beta^\dagger\} = 0$ and $\{\hat{\psi}_\alpha, \hat{\psi}_\beta^\dagger\} \in \mathbb{C}$, by defining

$$\bar{\mathcal{C}}_{\alpha\beta} = (\theta_{\alpha\succ\beta} - \theta_{k\succ l})\{\hat{\psi}_\alpha, \hat{\psi}_\beta^\dagger\}, \tag{46}$$

we observe that $\mathcal{C}_{\alpha\beta} = 0$ when α and β are both even or odd; $\mathcal{C}_{\alpha\beta} = \bar{\mathcal{C}}_{\alpha\beta}$ when α is odd and β is even; $\mathcal{C}_{\alpha\beta} = -\bar{\mathcal{C}}_{\alpha\beta}$ when α is even and β is odd. Therefore, we can express the GWT for fermionic fields as follows:

$$\mathcal{O}[F(\hat{\psi}, \hat{\psi}^\dagger)] = \mathcal{O}'[F(\hat{\psi}', \hat{\psi}'^\dagger)], \tag{47}$$

with

$$\hat{\psi}_\alpha' = \hat{\psi}_\alpha - \bar{\mathcal{C}}_{\alpha\beta}\partial_\beta^\dagger, \tag{48}$$

$$\hat{\psi}_\alpha'^\dagger = \hat{\psi}_\alpha^\dagger + \bar{\mathcal{C}}_{\alpha\beta}\partial_\beta\,. \tag{49}$$

If we identify $\mathcal{O} = \mathcal{T}$ and $\mathcal{O}' = \mathcal{N}$, we recover the form of fermionic Wick's theorem discussed in Refs. [6,7].

VI. EXAMPLES

In this section, we provide some applications of the GWT in order to show how this helps to tackle in a straightforward manner problems that possibly involve long calculations. Let us start by considering two generic bosonic operators $\hat{X}$, $\hat{Y}$, and the ordering $\mathcal{O}_{XY}$ that pushes the operator $\hat{X}$ to the left and the operator $\hat{Y}$ to the right, i.e.,

$$\mathcal{O}_{XY}[e^{\hat{X}+\hat{Y}}] = e^{\hat{X}}e^{\hat{Y}}. \tag{50}$$

We apply the GWT between $\mathcal{O}_{XY}$ and the Weyl ordering $\mathcal{W}$ defined by

$$\mathcal{W}[e^{\hat{X}+\hat{Y}}] = e^{\hat{X}+\hat{Y}}. \tag{51}$$

It is straightforward to show that the contraction (11) reads $\mathcal{C}_{XY} = (\mathcal{O}_{XY} - \mathcal{W})\hat{X}\hat{Y} = \frac{1}{2}[\hat{X}, \hat{Y}]$, and the GWT (38) predicts

$$e^{\hat{X}}e^{\hat{Y}} = e^{\hat{X}+\hat{Y}+\frac{1}{2}[\hat{X},\hat{Y}]}. \tag{52}$$

We thus see that the Baker-Campbell-Hausdorff (BCH) [24–26] formula for bosonic operators is a special instance of the GWT. This reverses the point of view taken in Ref. [22], where the tentative proof of GWT was based on the BCH formula, and therefore the GWT was understood to be a consequence of BCH, not its generalization.

Another interesting example is the application of the GWT to quadratic forms of the type $e^{\frac{1}{2}D_{\alpha\beta}\hat{\phi}_\alpha\hat{\phi}_\beta}$, which occur, e.g., in open quantum systems [27,28] and in quantum optics. For the special class where D is real positive (or negative), we are going to show that

$$\mathcal{O}\big[e^{\frac{1}{2}D_{\alpha\beta}\hat{\phi}_\alpha\hat{\phi}_\beta}\big] = \sqrt{|D'|/|D|}\,\mathcal{O}'\big[e^{\frac{1}{2}D'_{\alpha\beta}\hat{\phi}_\alpha\hat{\phi}_\beta}\big], \tag{53}$$

with $D'_{\alpha\beta} = (D^{-1}_{\alpha\beta} - \mathcal{C}_{\alpha\beta})^{-1}$, valid if $D' > 0$ (or negative when $D < 0$). We introduce the random real Gaussian variables ξ_α of zero mean $\boldsymbol{M}\xi_\alpha = 0$ and correlation $\boldsymbol{M}\xi_\alpha\xi_\beta = D_{\alpha\beta}$. The symbol $\boldsymbol{M}$ stands for the Gaussian integral

$$\boldsymbol{M}f(\xi_\alpha) \equiv \frac{1}{\sqrt{|D|}}\int f(\xi_\alpha)e^{-\frac{1}{2}D^{-1}_{\alpha\beta}\xi_\alpha\xi_\beta}\prod_{\alpha\in\Omega}\frac{d\xi_\alpha}{\sqrt{2\pi}}, \tag{54}$$

which allows us to write

$$\boldsymbol{M}e^{\xi_\alpha\hat{\phi}_\alpha} = e^{\frac{1}{2}D_{\alpha\beta}\hat{\phi}_\alpha\hat{\phi}_\beta}. \tag{55}$$

Then, using the GWT (38), we write

$$\begin{aligned} e^{\frac{1}{2}\mathcal{C}_{\alpha\beta}\partial_\alpha\partial_\beta}\mathcal{O}'\big[e^{\frac{1}{2}D_{\alpha\beta}\hat{\phi}_\alpha\hat{\phi}_\beta}\big] &= e^{\frac{1}{2}\mathcal{C}_{\alpha\beta}\partial_\alpha\partial_\beta}\boldsymbol{M}\mathcal{O}'[e^{\xi_\alpha\hat{\phi}_\alpha}] \\ &= \boldsymbol{M}\mathcal{O}'\big[e^{\frac{1}{2}\mathcal{C}_{\alpha\beta}\xi_\alpha\xi_\beta+\xi_\alpha\hat{\phi}_\alpha}\big], \end{aligned} \tag{56}$$

and performing the Gaussian integral according to (54) we eventually obtain Eq. (53). The proof for negative D is readily obtained by replacing ξ_α by $i\xi_\alpha$. In absence of the GWT, such a reordering of a quadratic form would require applying repeatedly the BCH formula on the lhs of Eq. (55), and resummation of the contributions obtained. It is thus clear that the GWT reduces the amount of calculations required.

The application of the GWT to the single-mode squeezing operator $e^{i\kappa\hat{q}\hat{p}}$, which is a special case of the previous example with D indefinite, was considered earlier in Refs. [22,29]. Here we calculate the $\mathcal{N}$-ordered form of the two-mode squeezing operator $\hat{S}(g) = \exp(g\hat{a}\hat{b} - \text{H.c.})$, where the emission operators of the two modes are $\hat{a}$, $\hat{b}$, respectively, and the squeezing parameter g can be chosen as non-negative. The main steps are similar as before, except we need two independent complex random Gaussians ξ_1, ξ_2, with correlations $\boldsymbol{M}|\xi_1|^2 = \boldsymbol{M}|\xi_2|^2 = g$ and $\boldsymbol{M}\xi_1^2 = \boldsymbol{M}\xi_2^2 = 0$. Then

$$\begin{aligned} \hat{S}(g) &= \boldsymbol{M}e^{(\xi_1\hat{a}+\xi_1^*\hat{b}+\xi_2\hat{a}^\dagger-\xi_2^*\hat{b}^\dagger)} \\ &= \boldsymbol{M}\mathcal{W}[e^{(\xi_1\hat{a}+\xi_1^*\hat{b}+\xi_2\hat{a}^\dagger-\xi_2^*\hat{b}^\dagger)}], \end{aligned} \tag{57}$$

where the second identity is simply given by the definition (51) of Weyl ordering. We can now apply the GWT (38) to write

$$\mathcal{W}[e^{(\xi_1\hat{a}+\xi_1^*\hat{b}+\xi_2\hat{a}^\dagger-\xi_2^*\hat{b}^\dagger)}] = \mathcal{N}\big[e^{\frac{1}{2}(\xi_1\xi_2-\xi_1^*\xi_2^*)}e^{(\xi_1\hat{a}+\xi_1^*\hat{b}+\xi_2\hat{a}^\dagger-\xi_2^*\hat{b}^\dagger)}\big], \tag{58}$$

where we exploited the fact that the only non-null contractions are $(\mathcal{W}-\mathcal{N})\hat{a}\hat{a}^\dagger = (\mathcal{W}-\mathcal{N})\hat{b}\hat{b}^\dagger = \frac{1}{2}$. By replacing this identity into Eq. (57) and performing the integration, we find the squeezing operator in normal ordering:

$$\hat{S}(g) = \sqrt{(g^2+1)}\,\mathcal{N}\big[e^{\frac{g}{g^2+1}[\hat{a}\hat{b}-\hat{b}^\dagger\hat{a}^\dagger-2g(\hat{a}^\dagger\hat{a}+\hat{b}^\dagger\hat{b}+1)]}\big]. \tag{59}$$

We remark that the same result might have been obtained directly from Eq. (53) by performing the suitable replacements.

We eventually mention that in a series of papers [19,30,31], Agarwal and Wolf set up a phase-space method to investigate, among other issues, expectation values of functions of creation and annihilation operators, ordered according to $\mathcal{W}$, $\mathcal{N}$, and $\mathcal{A}$ (antinormal ordering). The GWT allows us to recover and generalize this result, without the need to resort to the phase-space formalism. Namely, the GWT (41) allows us to write

$$\langle\mathcal{O}[F(\{\hat{a}_\gamma\}, \{\hat{a}_\gamma^\dagger\})]\rangle = \big\langle e^{\frac{1}{2}\mathcal{C}_{\alpha\beta}\partial_\alpha\partial_\beta^\dagger}\mathcal{O}'[F(\{\hat{a}_\gamma\}, \{\hat{a}_\gamma^\dagger\})]\big\rangle, \tag{60}$$

where the contraction is $\mathcal{C}_{\alpha\beta} = (\mathcal{O} - \mathcal{O}')\hat{a}_\alpha\hat{a}^\dagger_\beta$, and the derivatives are defined as $\partial_\alpha = \partial/\partial a_\alpha$ and $\partial^\dagger_\beta = \partial/\partial a^\dagger_\beta$. By recognizing that

$$(\mathcal{W} - \mathcal{N})\hat{a}_\alpha\hat{a}^\dagger_\beta = (\mathcal{A} - \mathcal{W})\hat{a}_\alpha\hat{a}^\dagger_\beta = \frac{1}{2}(\mathcal{A} - \mathcal{N})\hat{a}_\alpha\hat{a}^\dagger_\beta = \frac{\delta_{\alpha\beta}}{2}, \tag{61}$$

one recovers the results in Ref. [31].

VII. CONCLUSIONS

We have proven the general Wick's theorem, namely the generalization of Wick's theorem (which relates time ordering to normal ordering) to any pair of operator orderings. We have shown that the GWT has the same form both for bosonic and fermionic operators, i.e., those operators satisfying c-number (anti)commutation relations. As an application, we have demonstrated that the BCH formula for bosonic operators is a special instance of the GWT. We further considered the ordering of quadratic forms and we have shown that the GWT allows us to treat it in a rather straightforward manner, sensibly reducing the amount of calculations required with respect to earlier approaches. The relationship provided by the GWT is so general that it may possibly be applied in any field where operators ordering plays a role. Whether some form of GWT can be proven for operators satisfying general commutation relations is still an open issue, and it will be subject of future research.

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APPENDIX

In the main text, we make extensive use of derivative symbols to which special meanings are attached [6,7], and this Appendix aims to clarify their meaning and properties. The bosonic derivatives $\partial = \partial/\partial\phi$ used in Sec. IV should be understood as standard c-number derivatives. The action of $\partial/\partial\phi$ on a function of operators is thus equivalent to temporarily treating $\hat{\phi}$ like a c-number, then performing the derivative $\partial/\partial\phi$, and eventually restoring the hat on $\hat{\phi}$:

$$\frac{\partial}{\partial\phi}F(\hat{\phi}, \hat{\psi}, \ldots, \hat{\zeta}) = \frac{\partial}{\partial\phi}F(\phi, \hat{\psi}, \ldots, \hat{\zeta})\Big|_{\phi=\hat{\phi}}. \tag{A1}$$

As such, bosonic derivatives satisfy the following commutation relations:

$$[\partial_\alpha, \hat{\phi}_\beta] = \delta_{\alpha\beta}, \qquad [\partial_\alpha, \partial_\beta] = 0. \tag{A2}$$

Similarly, in Sec. V, where we are dealing with fermionic operators $\hat{\phi}$, the derivatives $\partial/\partial\phi$ should be understood as Grassmann derivatives, which satisfy

$$\{\partial_\alpha, \hat{\phi}_\beta\} = \delta_{\alpha\beta}, \qquad \{\partial_\alpha, \partial_\beta\} = 0. \tag{A3}$$

In order to perform the Grassmann derivative of a product of fermionic operators, one first needs to move the operator to be differentiated close to the derivative, by exploiting anti-commutation relations, and then the derivative can act as a standard c-number derivative:

$$\begin{aligned}\partial_{\alpha_j+1}\prod_i \hat{\phi}_{\alpha_i} &= (-1)^{n-j-1}\partial_{\alpha_j+1}\left(\hat{\phi}_{\alpha_{j+1}}\prod_{i\neq j+1}\hat{\phi}_{\alpha_i}\right)\\ &= (-1)^{n-j-1}\prod_{i\neq j+1}\hat{\phi}_{\alpha_i}.\end{aligned} \tag{A4}$$

This equation explains the term $(-1)^{n-j}$ in the second line of Eq. (44).

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