Normal Ordering and Composite Operators for Free Scalar Quantum Fields

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Abstract In quantum field theory, many models can be defined by treating spacetime as a very fine lattice, but operators that are well-defined on the lattice don't always remain well-defined in the continuous-spacetime limit. In some cases, we can fix this by smearing the operator over a region of spacetime that remains finite in the continuum limit, but in other cases the best we can do is construct operators whose n-point correlation functions remain well-defined as long as the points remain separated from each other in spacetime, even though the operators themselves do not remain well-defined as ordinary operators on the Hilbert space. The construction uses a prescription called **normal ordering**, which is a way of modifying the original operator to make its correlation functions well-defined in the continuum limit. This article introduces the concept and shows how to efficiently work out explicit expressions for the normal-ordered versions of arbitrary powers of a free scalar quantum field.

Contents

1 Introduction

Consider the free scalar quantum field in D-dimensional space (d-dimensional spacetime, with $d = D + 1$). Treat space as a lattice so that the field operator $\phi(\mathbf{x})$ at an individual point $\mathbf{x}$ is well-defined as an operator on the Hilbert space.[1] If $|0\rangle$ is the vacuum state, then $\phi(\mathbf{x})|0\rangle$ is another state-vector in the Hilbert space. Its norm

$$r \equiv \langle 0|\phi^2(\mathbf{x})|0\rangle \tag{1}$$

is a finite real number whose value will be estimated in section 8 as a function of the lattice spacing ϵ. In the continuous-space limit ($\epsilon \to 0$), the norm r becomes undefined ($r \to \infty$), which implies that $\phi(\mathbf{x})$ is not well-defined as an operator on the Hilbert space when space is continuous. In contrast, the **smeared** field operator

$$\phi(f) \equiv \epsilon^D \sum_{\mathbf{x}} f(\mathbf{x}, \epsilon)\phi(\mathbf{x})$$

does remain well-defined[2] if the function $f(\mathbf{x}, \epsilon)$ approaches a smooth function of nonzero width as $\epsilon \to 0$.

Squaring does not commute with smearing. In particular, even though $\phi^2(f)$ (the result of smearing-and-then-squaring $\phi(\mathbf{x})$) remains well-defined as an operator on the Hilbert space in the continuous-space limit, the combination

$$\int d^D x \; f(\mathbf{x})\phi^2(\mathbf{x}) \tag{2}$$

(the result of squaring-and-then-smearing $\phi(\mathbf{x})$) does not. This will be demonstrated in section 2. We can improve the behavior by subtracting its vacuum expectation value, because the correlation function

$$\big\langle 0\big|\big(\phi^2(\mathbf{x}) - r\big)\big(\phi^2(\mathbf{y}) - r\big)\big|0\big\rangle$$

[1] Article 52890

[2] In the infinite-volume limit, if the single-particle mass m is zero and space is one-dimensional ($D = 1$), then the smeared field operator becomes ill-defined (article 37301), but it remains well-defined if either $m > 0$ or $D \geq 2$ (or both).

has a well-defined continuum limit as long as $|\mathbf{x}-\mathbf{y}| > 0$. The combination $\phi^2(\mathbf{x})-r$ still doesn't have a well-defined continuum limit, not even if it's smeared over a finite region of space,[3] but it is still useful in many contexts where an ultraviolet cutoff (like the lattice spacing ϵ) is understood to be present. This is an example of a **composite operator**. More generally, composite operators are things whose n-point correlation functions (in the vacuum state) remain well-defined in the continuum limit, as long as the points remain separated from each other.[4] The behavior of such correlation functions as any two of the points approach each other is described by the **operator product expansion**[5]

$$\mathcal{O}_A(x)\mathcal{O}_B(y) \sim \sum_C w_{AB}^C(\mathbf{x}-\mathbf{y})\mathcal{O}_C(\mathbf{x}),$$

where each $\mathcal{O}_\bullet$ is a (composite) operator and the ws are complex-valued functions.

In general, just subtracting the vacuum expectation value is not sufficient: it is sufficient for the special case $\phi^2(\mathbf{x})$, but not for $\phi^n(\mathbf{x})$ when $n \geq 3$. To ensure that n-point correlation functions have well-defined continuum limits when the points are separated, we can use a prescription called **normal ordering**. One definition of *normal ordering* refers to the operator product expansion, specifically to the first nonsingular term in an expansion in powers of $|\mathbf{x}-\mathbf{y}|$. That definition is described in section 6.5 of Di Francesco *et al* (1997). This article uses another standard definition, one that refers to creation/annihilation operators instead of to the operator product expansion. This definition will be introduced in section 3.

[3] If it's smeared in both space and time, then it remains well-defined as an operator on the Hilbert space in the continuum limit if the number $d = D + 1$ of spacetime dimensions is $d \leq 3$ but not if $d \geq 4$ (section 2).

[4] A composite operator is not necessarily well-defined as an operator on the Hilbert space in the continuum limit, not even if it's smeared. The name *operator* is used more generally both in physics (where people often don't precisely define the symbols that they're manipulating) and in mathematics (because the elements of a $*$-algebra – defined in article 74088 – are often called *operators* even if they're not represented as linear operators on a Hilbert space).

[5] The convergence of this expansion in a particular model in four-dimensional spacetime is analyzed in Hollands *et al* (2014). Pappadopulo *et al* (2012) explores its convergence in CFTs (quantum field theories with conformal symmetry).

2 Composite operators in the continuum limit

Normal ordering will be defined more generally in section 3. Here is a special case of that definition: the normal ordered version of $\phi^2(x)$ is[6,7]

$$\Phi_2(x) \equiv \phi^2(x) - r \tag{3}$$

with r defined by (1). This section shows that $\Phi_2(x)$ cannot be a well-defined operator on the Hilbert space in the limit of continuous space(time) for most d, not even when smeared, even though it is well-defined when space(time) is treated with a lattice, even when not smeared. Two derivations will be given, one for a massless free scalar field smeared in spacetime, and one for a free scalar field with arbitrary mass smeared only in space.

First consider the case

$$\mathcal{O}_2 \equiv \int d^dx\ f(x)\Phi_2(x)$$

where $\phi(x)$ is a massless free scalar field in d-dimensional spacetime and the smearing function $f(x)$ has nonzero width in both the time and space dimensions. The massless free scalar field model has scale symmetry,[8] and the field $\phi(x)$ has scaling dimension[9] $(d-2)/2$, which means that when a scale symmetry transformation with scale factor λ is applied to $\phi(x)$, the result is $\lambda^{(d-2)/2}\phi(\lambda x)$. The vacuum state $|0\rangle$ is invariant under this symmetry, so equations (1) and (3) imply that $\Phi_2(x)$ has scaling dimension[10]

$$\Delta_2 = d - 2.$$

[6]The standard notation for the normal-ordered version of $\mathcal{O}(x)$ is $:\mathcal{O}(x):$. The non-standard notation used in this article is meant to make the equations easier to read.

[7]The symbol x denotes a point in spacetime. The boldface symbol $\mathbf{x}$ denotes a point in space.

[8]Article 09193

[9]Article 10142

[10]More generally, the definition of normal ordering introduced in section 6.5 of Di Francesco *et al* (1997) implies that if $\mathcal{O}_1$ and $\mathcal{O}_2$ have scaling dimensions Δ_1 and Δ_2, then their normal-ordered product has scaling dimension $\Delta_1 + \Delta_2$.

We can use this to show that the norm of the state-vector $\mathcal{O}_2|0\rangle$ diverges in the continuum limit when $d \geq 4$. Start with

$$\begin{aligned}\langle 0|\mathcal{O}_2\mathcal{O}_2|0\rangle &= \int d^dx\, d^dx'\ f(x)f(x')\langle 0|\Phi_2(x)\Phi_2(x')|0\rangle \\ &\propto \int d^dx\, d^dx'\ \frac{f(x)f(x')}{|x'-x|^{2\Delta_2}} \\ &= \int d^dx\, d^dx'\ \frac{f(x+x')f(x')}{|x|^{2\Delta_2}} \\ &= \int d^dx'\ f(x')\int d^dx\ \frac{f(x+x')}{|x|^{2\Delta_2}}.\end{aligned}$$

The fact that $\Phi_2(x)$ has scaling dimension Δ_2 was used to get the second line. If B is any small neighborhood of the point $x = 0$, then the integral

$$\int_B d^dx\ \frac{1}{|x|^{2\Delta_2}} \propto \int_B s^{d-1}ds\ \frac{1}{s^{2\Delta_2}} \qquad\qquad \big(s \equiv |x|\big)$$

is undefined when $d - 1 - 2\Delta_2 < 0$, so the norm of $\mathcal{O}_2|0\rangle$ is undefined when $d \geq 4$, as claimed.

The same conclusion should hold even if the mass m is nonzero, because the divergence comes from the limit $\epsilon \to 0$, and m should be made negligible when expressed in units of $1/\epsilon$ so that m remains finite when $\epsilon \to 0$.

Now recycle the symbol $\mathcal{O}_2$ and consider the case

$$\mathcal{O}_2 \equiv \int d^Dx\ f(\mathbf{x})\Phi_2(\mathbf{x}),$$

where $\phi(\mathbf{x}) \equiv \phi(\mathbf{x}, t = 0)$ is a free scalar field in D-dimensional space, not necessarily massless, $\Phi_2(x)$ is the normal-ordered version of $\phi^2(x)$, and the smearing is only in the spatial dimensions. Use the expression for $\phi(\mathbf{x})$ from article 00980 to get

$$\Phi_2(\mathbf{x})|0\rangle \propto \int d^Dp_1\, d^Dp_2\ \frac{a^\dagger(\mathbf{p}_1)a^\dagger(\mathbf{p}_2)e^{-i(\mathbf{p}_1+\mathbf{p}_2)\cdot\mathbf{x}}}{\sqrt{\omega(\mathbf{p}_1)\omega(\mathbf{p}_2)}}.$$

Together with the identity

$$\langle 0|a(\mathbf{p}_1')a(\mathbf{p}_2')a^\dagger(\mathbf{p}_1)a^\dagger(\mathbf{p}_2)|0\rangle \propto \delta(\mathbf{p}_1'-\mathbf{p}_1)\delta(\mathbf{p}_2'-\mathbf{p}_2)+\delta(\mathbf{p}_1'-\mathbf{p}_2)\delta(\mathbf{p}_2'-\mathbf{p}_1)$$

and the abbreviation

$$G(\mathbf{x}'-\mathbf{x}) \equiv \langle 0|\Phi_2(\mathbf{x})\,\Phi_2(\mathbf{x}')|0\rangle,$$

this implies

$$\begin{aligned}\int d^Dx\,d^Dx'\;f(\mathbf{x})f(\mathbf{x}')G(\mathbf{x}'-\mathbf{x}) &\propto \int d^Dx\,d^Dx'\;f(\mathbf{x})f(\mathbf{x}')\int d^Dp_1\,d^Dp_2\;\frac{e^{i(\mathbf{p}_1+\mathbf{p}_2)\cdot(\mathbf{x}'-\mathbf{x})}}{\sqrt{\omega(\mathbf{p}_1)\omega(\mathbf{p}_2)}}\\ &\propto \int d^Dx\,d^Dx'\;f(\mathbf{x}+\mathbf{x}')f(\mathbf{x}')\int d^Dp_1\,d^Dp_2\;\frac{e^{-i(\mathbf{p}_1+\mathbf{p}_2)\cdot\mathbf{x}}}{\sqrt{\omega(\mathbf{p}_1)\omega(\mathbf{p}_2)}}.\end{aligned}$$

But

$$\int d^Dp_1\,d^Dp_2\;\frac{e^{-i(\mathbf{p}_1+\mathbf{p}_2)\cdot(\mathbf{x})}}{\sqrt{\omega(\mathbf{p}_1)\omega(\mathbf{p}_2)}} \sim |\mathbf{x}|^{1-2D}$$

so the norm of $\mathcal{O}_2|0\rangle$ is undefined if $D\geq 1$ (that is, if $d\geq 2$). This confirms that smearing in only the spatial dimensions is even less effective than smearing in both the space and time dimensions.

Extending either of these methods to ϕ^n shows that the divergence is even worse when the exponent n is larger.

3 Normal ordering

This section gives the general definition of normal ordering that will be used in the rest of this article. Choose a point x in spacetime and use the abbreviation

$$\phi \equiv \phi(x).$$

Write

$$\phi = C + A$$

where C is the adjoint of A, and $A|0\rangle = 0$. Mnemonic: C is the creation-operator part of ϕ, and A is the annihilation-operator part of ϕ. The commutator

$$r \equiv [A, C] \equiv AC - CA = \frac{\langle 0|\phi^2|0\rangle}{\langle 0|0\rangle}$$

is a positive real number.[11,12] Define Φ_n to be the operator obtained from the formal expression $(C + A)^n$ by writing all factors of C to the left of all factors of A in each term.[13] Example:

$$\Phi_2 = C^2 + 2CA + A^2.$$

The goal is to derive an expression for Φ_n as a polynomial in ϕ. Section 5 will show a few examples, and section 7 will show another way of writing them.

[11] This is only true in a model without any interactions. This article is limited to *free* scalar quantum fields.

[12] Section 8 estimates the value of this number when D-dimensional space is treated as an infinite lattice.

[13] The motive for this definition is the fact that $\Phi_n(x)$ (the normal ordered version of $\phi^n(x)$) has well-defined vacuum correlation functions in the continuum limit, as long as the points are all distinct from each other.

4 The key identity

The key identity is[14]

$$\boxed{\Phi_n = \phi\Phi_{n-1} - (n-1)r\Phi_{n-2}.} \tag{4}$$

To derive this, start with the obvious identity

$$\phi\Phi_{n-1} = C\Phi_{n-1} + \Phi_{n-1}A + \big[A, \Phi_{n-1}\big],$$

which may also be written

$$\phi\Phi_{n-1} = \Phi_n + \big[A, \Phi_{n-1}\big]. \tag{5}$$

Now use the identity

$$[A, C^k] = krC^{k-1}$$

to see that $[A, \cdots]$ acts formally like r times the derivative with respect to C:

$$[A, \cdots] \sim r\frac{\partial}{\partial C}\cdots .$$

Use this in (5) to get (4).

[14] Brunetti *et al* (1996) uses a more general version of this as the *definition* of normal ordering (definition 5.1 in that paper), but they express the definition in terms of $\phi(x_1)\cdots\phi(x_n)$ instead of $\phi^n(x)$ because they work directly in continuous spacetime. Then they define a normal-ordered version of $\phi^n(f)$ (they call it a **Wick monomial**), where $\phi(f)$ is the smeared field operator $\int f(x)\phi(x)$. This is expressed more concisely but less explicitly by equation (7) in the preprint version of Pinamonti (2008). Their approach is explored further in Hollands and Ruan (2002).

5 Results

For $n = 2$, the key identity (4) reduces to

$$\boxed{\Phi_2 = \phi^2 - r.} \tag{6}$$

For $n = 3$, the key identity (4) reduces to

$$\Phi_3 = \phi\Phi_2 - 2r\phi.$$

Use (6) in the right-hand side to get

$$\boxed{\Phi_3 = \phi^3 - 3r\phi.} \tag{7}$$

For $n = 4$, the key identity (4) reduces to

$$\Phi_4 = \phi\Phi_3 - 3r\Phi_2.$$

Use (6) and (7) in the right-hand side to get

$$\boxed{\Phi_4 = \phi^4 - 6r\phi^2 + 3r^2 = (\phi^2 - 3r)^2 - 6r^2.} \tag{8}$$

Similarly,

$$\begin{aligned}
\Phi_5 &= \phi^5 - 10r\phi^3 + 15r^2\phi \\
\Phi_6 &= \phi^6 - 15r\phi^4 + 45r^2\phi^2 - 15r^3 \\
\Phi_7 &= \phi^7 - 21r\phi^5 + 105r^2\phi^3 - 105r^3\phi \\
\Phi_8 &= \phi^8 - 28r\phi^6 + 210r^2\phi^4 - 420r^3\phi^2 + 105r^4.
\end{aligned}$$

6 Relationship to Bell polynomials

The **Bell polynomial** $B_n(a_1, ..., a_n)$ is defined by the condition[15]

$$\sum_{n=0}^{\infty} \frac{1}{n!} B_n(a_1, ..., a_n) z^n = \exp\left(\sum_{n=1}^{\infty} \frac{1}{n!} a_n z^n\right). \tag{9}$$

This section shows that Φ_n can be written[16]

$$\Phi_n = B_n(\phi, -r, 0, ..., 0). \tag{10}$$

Use (10) in (9) to get

$$\sum_{n=0}^{\infty} \frac{1}{n!} \Phi_n z^n = \exp\left(\phi z - \frac{r}{2} z^2\right), \tag{11}$$

which may also be written

$$\boxed{\Phi_n = \left(\frac{d}{dz}\right)^n \exp\left(\phi z - \frac{r}{2} z^2\right)\bigg|_{z=0}.} \tag{12}$$

Use the identity

$$\left(\frac{d}{dz}\right)^n \exp\left(\phi z - \frac{r}{2} z^2\right) = \left(\frac{d}{dz}\right)^{n-1} \left((\phi - rz) \exp\left(\phi z - \frac{r}{2} z^2\right)\right)$$

to deduce that (12) implies (4).

[15]The study of relationships like this is called **umbral calculus** (Roman and Rota (1978)). Some references are linked in https://ncatlab.org/nlab/show/umbral+calculus.

[16]This is stated without proof in Ellis *et al* (2016).

7 Another way to write the results

The generating function (11) can also be written

$$\boxed{\sum_{n=0}^{\infty} \frac{1}{n!}\Phi_n z^n = \exp(\phi z)\exp\left(-\frac{r}{2}z^2\right).} \tag{13}$$

Expand the right-hand side in powers of z to get

$$\begin{aligned}
\frac{1}{4!}\Phi_4 &= \frac{\phi^4}{4!} - \left(\frac{r}{2}\right)\frac{\phi^2}{2!} + \text{const} \\
\frac{1}{6!}\Phi_6 &= \frac{\phi^6}{6!} - \left(\frac{r}{2}\right)\frac{\phi^4}{4!} + \frac{1}{2}\left(\frac{r}{2}\right)^2\frac{\phi^2}{2!} + \text{const} \\
\frac{1}{8!}\Phi_8 &= \frac{\phi^8}{8!} - \left(\frac{r}{2}\right)\frac{\phi^6}{6!} + \frac{1}{2}\left(\frac{r}{2}\right)^2\frac{\phi^4}{4!} - \frac{1}{3!}\left(\frac{r}{2}\right)^3\frac{\phi^2}{2!} + \text{const}
\end{aligned}$$

and so on. These should be compared to the expressions derived in article 79649 for the eigenfunctions of the linearized renormalization group equations.

8 Evaluating r

Use the same formulation and notation as article 00980, treating D-dimensional space as a lattice of infinite size. In the massless version of the model with $D \geq 2$,[17] the constant r defined in sections 1 and 3 is

$$r = \int \frac{d^D p}{(2\pi)^D} \, \frac{1}{2\omega(\mathbf{p})} \tag{14}$$

with

$$\omega(\mathbf{p}) \equiv \sqrt{\sum_k \left(\frac{2\sin(\mathbf{e}_k \cdot \mathbf{p}/2)}{\epsilon}\right)^2}.$$

The domain of integration is the Brillouin zone (article 71852)

$$|p_k| \leq \frac{\pi}{\epsilon}.$$

Instead of trying to evaluate the integral (14) exactly, this section derives easy upper and lower bounds. The inequalities

$$\frac{2\theta}{\pi} \leq \sin\theta \leq \theta$$

hold for all $0 \leq \theta \leq \pi/2$, which implies

$$\rho \leq r \leq \frac{\pi}{2}\rho \tag{15}$$

with[18]

$$\rho \equiv \int \frac{d^D p}{(2\pi)^D} \, \frac{1}{2|\mathbf{p}|} \qquad\qquad |\mathbf{p}| \equiv \sqrt{\sum_k p_k^2}. \tag{16}$$

[17]For $D = 1$, the integral (14) is undefined when the lattice has infinite size. Article 37301 explains how to modify the model so that this doesn't cause any problems.

[18]Equation (2.125) in Repko (2016) shows the exact value of the integral (16) when $D = 3$, but without the factor of $2(2\pi)^D$ in the denominator. After adjusting for that factor, the result in Repko (2016) gives $\rho \approx 0.189$.

The domain of integration is a D-dimensional cube with edge-length $2\pi/\epsilon$. Define ρ_0 to be the integral with the same integrand but whose domain is the largest sphere contained within that cube. Define ρ_1 to be the integral with the original domain of integration but with the integrand replaced by $\epsilon/(2\pi)$ wherever $|\mathbf{p}| > \pi/\epsilon$. Then

$$\rho_0 \leq \rho \leq \rho_1. \tag{17}$$

The integrals ρ_0 and ρ_1 are both easy to evaluate. Define Ω_D by the relationship

$$\rho_0 = \frac{\Omega_D}{(2\pi)^D}\int_0^{\pi/\epsilon}\frac{p^{D-1}dp}{2p}.$$

In words, Ω_D is the D-dimensional version of the "surface area" of the unit sphere. (Examples: $\Omega_2 = 2\pi$ and $\Omega_3 = 4\pi$.) Then

$$\rho_0 = \frac{\Omega_D}{(2\pi)^D}\frac{(\pi/\epsilon)^{D-1}}{2(D-1)}$$

and[19]

$$\rho_1 = \rho_0 + \frac{\epsilon/(2\pi)}{(2\pi)^D}\left((2\pi/\epsilon)^D - \Omega_D\frac{(\pi/\epsilon)^D}{D}\right).$$

Combine (15) and (17) to get the final result

$$\boxed{\rho_0 \leq r \leq \frac{\pi}{2}\rho_1.}$$

When $D = 3$, this becomes

$$\frac{1}{8\epsilon^2} \leq r \leq \frac{1}{4\epsilon^2}\left(\frac{\pi}{12}+1\right).$$

[19]The first term in large parentheses is the volume of the cube with edge-length $2\pi/\epsilon$, and the second term is the volume of the sphere with radius π/ϵ.

9 References

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