Contour Integrals: Applications to the Free Scalar Model

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Abstract As a technical supplement to articles 00980 and 30983, this article explains how contour integrals may be used to estimate the large-distance behavior of some functions that arise in the analysis of the free scalar quantum field on a spatial lattice.

Contents

1 Motivation

In quantum field theory (QFT), a relatively straightforward way to construct some models without any mathematical ambiguity involves treating space as a very large and very fine lattice. Articles 00980 and 30983 apply this approach to a simple model involving only a free scalar field $\phi(\mathbf{x}, t)$, where $\mathbf{x} = (x_1, ..., x_D)$ is a point in D-dimensional space and t is the time coordinate.[1] Many QFT textbooks explain how to derive the result[2]

$$\langle 0|\phi(\mathbf{x}, t)\phi(\mathbf{y}, t)|0\rangle \sim e^{-m|\mathbf{x}-\mathbf{y}|},$$

where $|0\rangle$ is the vacuum state and m is the single-particle mass, but they usually start in continuous space where the "operator" $\phi(\mathbf{x}, t)$ is not really well-defined. This article explains how to derive this result – and other related results – when space is treated as a lattice, so that $\phi(\mathbf{x}, t)$ is perfectly well-defined as an operator on (a dense subset of) the Hilbert space.

The free scalar model can be defined directly in continuous space, as explained in article 44563, but most QFT textbooks don't use that approach because it doesn't generalize to nontrivial models. The lattice approach does, but most traditional QFT textbooks don't start with the lattice approach, either, because it's messy and artificial. The net result is that most traditional QFT textbooks don't actually define their models at all, which can make the whole subject seem ad-hoc. The message in this article is that the same results may be derived in a legitimate way from a clearly-defined model, so the subject really does have (or really can be given) a solid foundation.[3]

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[1] This article uses the same notation as in those articles, including $\mathbf{p}\cdot\mathbf{x} \equiv \sum_n p_n x_n$ and $\mathbf{x}^2 \equiv \mathbf{x}\cdot\mathbf{x}$ and $|\mathbf{x}| \equiv \sqrt{\mathbf{x}\cdot\mathbf{x}}$, but here the lattice has infinite size, so $\int d^D p\ \cdots$ really is an integral (not a sum). The integral is over a Brillouin zone, as explained in article 71852.

[2] Examples include page 27 in Peskin and Schroeder (1995) and page 35 in Itzykson and Zuber (1980).

[3] The message is that using a lattice is *one* way to define models in QFT, not that it's the "right" way. It clearly can't be the "right" way, because lattice-based definitions are never unique: many models that differ in their details at the lattice scale become indistinguishable from each other in the (near-)continuum limit. We do not yet know the "right" way to define models in QFT (Tachikawa (2017)), not even if we only consider those models for which a nontrivial strict continuum limit probably does exist.

2 The quantities of interest

When the free scalar model is defined on a spatial lattice, as in articles 00980 and 30983, the infinite-volume limit of the equal-time two-point vacuum correlation function is

$$\langle 0|\phi(\mathbf{x},t)\phi(\mathbf{y},t)|0\rangle \propto \int_{\text{B.Z.}} \frac{d^D p}{(2\pi)^D}\;\frac{e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}}{\sqrt{m^2+\hat{\mathbf{p}}^2}} \tag{1}$$

where the integral is over each component of $\mathbf{p}$ from $-\pi/\epsilon$ to π/ϵ, where ϵ is the distance between neighboring lattice sites, and the components of $\hat{\mathbf{p}}$ are

$$\hat{p}_n \equiv \frac{\sin(p_n\epsilon/2)}{\epsilon/2}.$$

The subscript "B.Z." stands for Brillouin zone, a reminder that this is the domain of integration (article 71852). The constant m is a positive real number ($m > 0$), and each component of $\mathbf{x}$ or $\mathbf{y}$ is an integer multiple of the lattice spacing ϵ. More generally, analysis of the free scalar model involves various functions of the form

$$f_n(\mathbf{x}-\mathbf{y}) \equiv \int_{\text{B.Z.}} \frac{d^D p}{(2\pi)^D}\; e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}\left(m^2+\hat{\mathbf{p}}^2\right)^{1/n}, \tag{2}$$

where n is a nonzero integer (positive or negative). The goal is to deduce something about how quickly this function approaches zero as the distance $|\mathbf{x}-\mathbf{y}|$ increases.

The integral (2) is clearly well-defined, because the integrand and the domain of integration are both finite, but it's inconvenient as it stands because the quantity $\hat{\mathbf{p}}^2$ is not isotropic (symmetric under rotations) as a function of $\mathbf{p}$. We only care about the continuum limit $\epsilon \to 0$, in which this asymmetry disappears. In that limit, the domain of integration becomes infinite and the integral is not absolutely convergent.[4] In fact, for $\mathbf{x} = \mathbf{y}$, the integral (2) does *not* remain finite in the continuum limit.[5] The remaining sections explain how to evaluate the continuum limit of (2) when the distance $|\mathbf{x}-\mathbf{y}|$ is held fixed at a finite nonzero value.

[4]An integral $\int ds\; f(s)$ is called **absolutely convergent** if $\int ds\; |f(s)|$ is finite.

[5]This is related to the fact that, in the continuum limit, $\phi(\mathbf{x},t)$ is not well-defined as an operator on the Hilbert space.

3 Strategy

To evaluate (2), the strategy will be to write it as a sum of two terms, one that has rotation symmetry and one that goes to zero in the continuum limit. The domain of integration in (2) is the D-dimensional analog of a cube: each of the D integration variables goes from $-\pi/\epsilon$ to π/ϵ, independently of the others. Choose a ϵ-independent constant λ such that

$$0 < \lambda \ll 1, \tag{3}$$

and use the abbreviation

$$\Lambda \equiv \frac{\lambda}{\epsilon}.$$

Separate the domain of integration into two parts, one of which is defined by the rotation-symmetric condition $\mathbf{p}^2 < \Lambda^2$. The quantity (2) may be written

$$f_n(\mathbf{x}-\mathbf{y}) = \int_{\mathbf{p}^2<\Lambda^2} \frac{d^Dp}{(2\pi)^D}\; e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})} \left(m^2+\hat{\mathbf{p}}^2\right)^{1/n} + \text{remainder}. \tag{4}$$

In the first term, the condition (3) implies

$$\hat{\mathbf{p}}^2 \approx \mathbf{p}^2.$$

We can make this approximation arbitrarily good by making λ arbitrarily small, as long as λ is nonzero and is held fixed when we take the limit $\epsilon \to 0$. Using this arbitrarily-good approximation, the first term in (4) becomes $f_{n,\Lambda}(\mathbf{x}-\mathbf{y})$ with

$$f_{n,\Lambda}(\mathbf{x}) \equiv \int_{\mathbf{p}^2<\Lambda^2} \frac{d^Dp}{(2\pi)^D}\; e^{i\mathbf{p}\cdot\mathbf{x}} \left(m^2+\mathbf{p}^2\right)^{1/n}. \tag{5}$$

Section 6 shows how to evaluate the continuum limit of this integral, and section 7 will show that the remainder in (4) goes to zero in the continuum limit.

4 A quick review of contour integrals

Let C be a curve (also called a **contour**) in the complex plane, described by a complex-valued function $z(s)$ of a real variable s. If the curve $z(s)$ is smooth except at a finite number of points, then the **contour integral** of a function $f(z)$ along the curve C is defined by

$$\int_C dz\ f(z) \equiv \int ds\ \frac{dz(s)}{ds} f\big(z(s)\big).$$

As an example, consider the curve defined by $z(\theta) \equiv e^{i\theta}$ for $0 \leq \theta < 2\pi$, and let f be the function $f(z) \equiv 1/z$. Then

$$\int_C dz\ \frac{1}{z} = \int_0^{2\pi} d\theta\ ie^{i\theta}\,\frac{1}{e^{i\theta}} = i\int_0^{2\pi} d\theta = 2\pi i.$$

A function $f(z)$ of a complex variable z is called **holomorphic** if its derivative with respect to z,

$$\frac{df}{dz} \equiv \lim_{\Delta z\to 0} \frac{f(z+\Delta z) - f(z)}{\Delta z}$$

is independent of the direction along which the limit is taken in the complex plane. A function $f(z)$ if holomorphic if and only if it is **analytic**,[6] so these names can both be used for the same class of functions. One of the most important facts about contour integrals is **Cauchy's integral theorem**, which says that if a function $f(z)$ is holomorphic in a simply-connected region R of the complex plane with boundary ∂R, then the contour integral of $f(z)$ around ∂R is zero:

$$\int_{\partial R} dz\ f(z) = 0 \qquad\qquad \text{if } f \text{ is holomorphic in } R.$$

[6] Both are defined in Rao *et al* (2015), section 2.1, where their equivalence is also previewed.

5 Where is an nth root analytic?

Let n be an integer with $|n| \geq 2$. When z is allowed to be complex-valued, the expression $z^{1/n}$ is ambiguous, because the condition $w^n = z$ is equivalent to the condition $(we^{2\pi i/n})^n = z$. One way to resolve the ambiguity is to require the phase θ in $z^{1/n} = |z^{1/n}|\, e^{i\theta}$ to satisfy

$$\theta_0 < \theta \leq \theta_0 + \frac{2\pi}{n} \tag{6}$$

for some arbitrary fixed value of θ_0. This makes $z^{1/n}$ unambiguous. With this definition, $z^{1/n}$ is an analytic (equivalently, holomorphic) function of z everywhere *except* along the half-line $z = |z|\, e^{in\theta_0}$. This half-line is called a **branch cut**. A branch cut is a discontinuity that was introduced to eliminate what would have otherwise been an ambiguity.

Now let ω be any real-valued positive constant. When p is allowed to be complex-valued, the expression $(p^2 + \omega^2)^{1/n}$ is again ambiguous, but we can resolve the ambiguity by requiring

$$(p^2 + \omega^2)^{1/n} = \big|(p^2 + \omega^2)^{1/n}\big|\, e^{i\theta}$$

where θ_0 satisfies (6) for some arbitrary fixed value of θ_0. Then $(p^2 + \omega^2)^{1/n}$ is an analytic function of p everywhere *except* along the branch cut

$$p^2 + \omega^2 = \big|p^2 + \omega^2\big|\, e^{in\theta_0}. \tag{7}$$

Where in the complex p-plane is this branch cut located? As an example, suppose we choose $\theta_0 = -\pi/n$, so that the equation for the branch cut becomes

$$p^2 + \omega^2 = -\big|p^2 + \omega^2\big|. \tag{8}$$

This equation cannot be satisfied unless p^2 is a negative real number, in which case (8) says that its magnitude must satisfy $|p^2| - \omega^2 = \big||p^2| - \omega^2\big|$. Altogether, the branch cut (8) consists of those complex values of p whose real part is zero and whose magnitude is $\geq \omega$.

6 Evaluating the rotation-symmetric term

The function (5) is invariant under rotations, because a rotation of the argument $\mathbf{x}$ can be cancelled by a rotation of the integration variable $\mathbf{p}$ in the exponential factor. (Everything else about the integral is invariant under rotations of $\mathbf{p}$.) To evaluate the integral (5), rotate the coordinate system so that $\mathbf{x}$ has only one nonzero component, say $\mathbf{x} = (x, 0, 0, ..., 0)$. Let p denote the first component of $\mathbf{p}$, and denote the remaining $D-1$ components collectively by $\overline{\mathbf{p}}$. With this notation, the integral (5) may be written

$$f_{n,\Lambda}(\mathbf{x}) \propto \int_{\overline{\mathbf{p}}^2<\Lambda^2} d^{D-1}\overline{p}\ g_{n,\Lambda}(\overline{\mathbf{p}}, x) \tag{9}$$

with

$$g_{n,\Lambda}(\overline{\mathbf{p}}, x) \equiv \int_{p^2<\Lambda^2-\overline{\mathbf{p}}^2} dp\ e^{ipx}\,(p^2+\omega^2(\overline{\mathbf{p}}))^{1/n} \tag{10}$$

and

$$\omega(\overline{\mathbf{p}}) \equiv \sqrt{m^2+\overline{\mathbf{p}}^2}.$$

For $|n| \geq 2$, the large-$|x|$ behavior of the function (10) can be determined using Cauchy's integral theorem. To do this, define $(p^2+\omega^2(\overline{\mathbf{p}}))^{1/n}$ as in section 5, with the branch cut given by equation (8). Then the integrand of (10) is an analytic function of p everywhere in the complex plane except along the two half-lines where its real part is zero and its magnitude is $\geq \omega(\overline{\mathbf{p}})$. This implies

$$\int_C dp\ e^{ipx}\,(p^2+\omega^2(\overline{\mathbf{p}}))^{1/n} = 0 \tag{11}$$

for any contour C that does not cross either of those half-lines. One example of such a contour is shown in figure 1. We can take part of the contour to run along the real axis from $-\sqrt{\Lambda^2-\overline{\mathbf{p}}^2}$ to $\sqrt{\Lambda^2-\overline{\mathbf{p}}^2}$, and we can take the return path to be a semicircle with a notch along the imaginary axis to avoid the branch cut, as

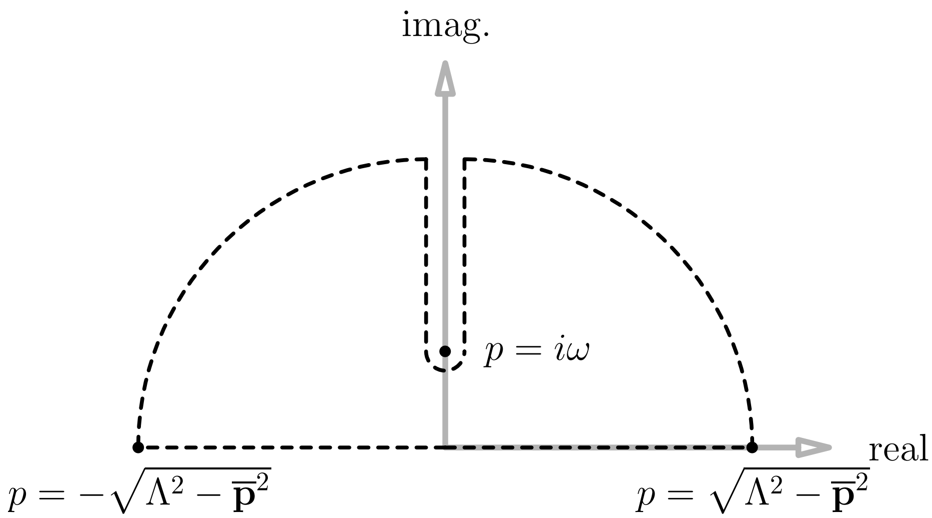

Figure 1 – Example of a contour inside which the integrand of (10) is an analytic function of the complex variable p.

shown in the figure. If $x > 0$, then the return path should be in the upper half-plane, where the imaginary part of p is positive. If $x < 0$, then the return path should be in the lower half-plane, where the imaginary part of p is negative. Either way, for any given $x \neq 0$, the value of the exponential factor e^{ipx} goes to zero as $e^{-|px|}$ when $|p| \to \infty$, so taking the continuum limit $\Lambda \to \infty$ reduces equation (11) to

$$\int_{\mathbb{R}} dp\ e^{ipx}\,\big(p^2 + \omega^2(\overline{\mathbf{p}})\big)^{1/n} + \int_{\text{notch}} dp\ e^{ipx}\,\big(p^2 + \omega^2(\overline{\mathbf{p}})\big)^{1/n} = 0$$

where the first integral is along the whole real axis and the second integral is along the notch that avoids the branch cut. The notch has two parts: one that descends down from $+i\infty$ (or ascends up from $-i\infty$) along one face of the branch cut, and another that ascends back toward $+i\infty$ (or descends back toward $-i\infty$) along the other face of the branch cut. These two parts are equal to[7]

$$\pm e^{\pm i\pi/n}\int_{\omega(\overline{\mathbf{p}})}^{\infty} dr\; e^{-\omega(\overline{\mathbf{p}})r}(\omega^2(\overline{\mathbf{p}})-r^2)^{1/n},$$

respectively, so the preceding equation gives

$$\int_{\mathbb{R}} dp\; e^{ipx}\,(p^2+\omega^2(\overline{\mathbf{p}}))^{1/n} \propto (e^{i\pi/n}-e^{-i\pi/n})\int_{\omega(\overline{\mathbf{p}})}^{\infty} dr\; e^{-rx}(\omega^2(\overline{\mathbf{p}})-r^2)^{1/n}.$$

Thanks to the exponentially-decreasing factor in the integrand, this is a manifestly finite expression for the $\Lambda\to\infty$ limit of the function $g_{n,\Lambda}$ defined in (10). Use this in (9) to get this expression for the continuum limit of (5):

$$\lim_{\Lambda\to\infty} f_{n,\Lambda}(\mathbf{x}) \propto (e^{i\pi/n}-e^{-i\pi/n})\int d^{D-1}\overline{p}\;\int_{\omega(\overline{\mathbf{p}})}^{\infty} dr\; e^{-r|\mathbf{x}|}(\omega^2(\overline{\mathbf{p}})-r^2)^{1/n}. \tag{12}$$

This function decreases asymptotically as $\sim e^{-m|\mathbf{x}|}$. According to equation (1), the special case $n=-2$ is the result that was quoted in section 1.

The contour-integration method used here has an implication that might be surprising at first. If the factor of $(m^2+\mathbf{p}^2)^{1/n}$ in equation (5) were replaced with a polynomial function of $\mathbf{p}$, then the integrand would be analytic everywhere, so the contributions from the two sides of the notch would cancel each other (or the notch could be eliminated), and so the integral would be zero for all $\mathbf{x}\neq\mathbf{0}$. Article 58590 introduces a different perspective in which this outcome isn't surprising at all.

[7]The factors of $e^{\pm i\pi/n}$ come from choosing θ_0 as in section 5.

7 Evaluating the remainder

This section shows that if $|\mathbf{x}| > 0$, then the remainder-term in equation (4) goes to zero in the continuum limit, leaving only the rotation-symmetric term (5) that was evaluated in section 6. The remainder in (4) is

$$R_n(\mathbf{x}) = \int_{\mathbf{p}^2>\Lambda^2,\ \text{B.Z.}} \frac{d^D p}{(2\pi)^D}\ e^{i\mathbf{p}\cdot\mathbf{x}} \left(m^2 + \hat{\mathbf{p}}^2\right)^{1/n} \tag{13}$$

where the integral is over all $\mathbf{p}$ in the Brillouin zone excluding those with $\mathbf{p}^2 < \Lambda^2$. Write the integral over $\mathbf{p}$ as an integral over the magnitude $p \equiv |\mathbf{p}|$ followed by an integral over the direction of $\mathbf{p}$. The lower limit of the integral over p is Λ. The upper limit depends on the direction of $\mathbf{p}$ because the Brillouin zone is not rotationally symmetric. Explicitly, the integral over the magnitude p is proportional to

$$\int_\Lambda^\Gamma dp\ e^{ip|\mathbf{x}|\cos\theta} \left(m^2 + \hat{\mathbf{p}}^2\right)^{1/n}, \tag{14}$$

where the upper limit Γ depends on the direction of $\mathbf{p}$. The quantity $\hat{\mathbf{p}}^2$ may be written more explicitly as

$$\hat{\mathbf{p}}^2 = \sum_n \frac{2 - e^{ipa_n\epsilon} - e^{-ipa_n\epsilon}}{\epsilon^2}$$

where each a_n is a direction-dependent factor between -1 and 1. This shows that $\hat{\mathbf{p}}^2$ is an analytic function of p with a magnitude that increases monotonically[8] with increasing $|p|$, so the factor $\left(m^2 + \hat{\mathbf{p}}^2\right)^{1/n}$ is an analytic function of p except along a pair of branch cuts that we can take to be on the imaginary-p axis, as before. Exactly how closely these branch cuts approach the origin depends on the direction parameters a_n. Now, let C be a contour that runs along the real axis from Λ to Γ, then traces out an arc with radius $|p| = \Gamma$ in the complex p-plane (either in the

[8] To prove this, take the derivative with respect to p and recall that $\mathbf{p}$ is restricted to the Brillouin zone.

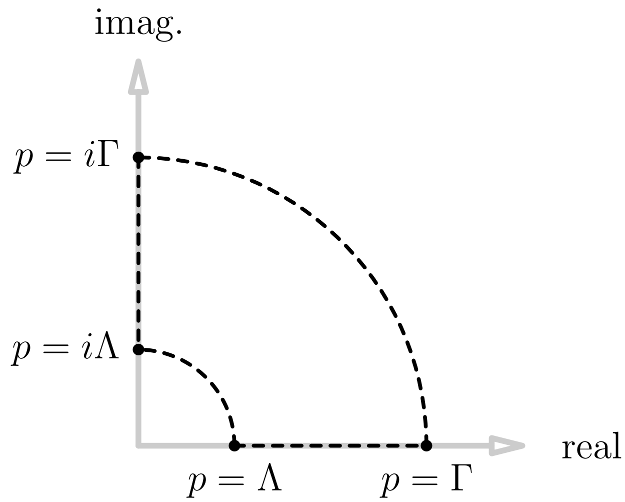

Figure 2 – Example of a contour inside which the integrand of (14) is an analytic function of p. In this example, the contour reaches all the way to the branch cut (which is as far as it's allowed to go), but that's not necessary. Any excursion away from the real axis would be sufficient.

upper or lower half-plane, depending on the sign of $\cos\theta$ in the exponent of (14)), stops before it crosses the branch cut, then runs radially back toward the origin until $|p| = \Lambda$, then traces out an arc with radius Λ until it meets the real axis again, closing the contour. This is depicted in figure 2. The integrand of (14) is analytic everywhere inside this contour, so Cauchy's integral theorem gives

$$\int_C dp\; e^{ip|\mathbf{x}|\cos\theta}\left(m^2 + \hat{\mathbf{p}}^2\right)^{1/n} = 0. \tag{15}$$

In the continuum limit $\Lambda \to \infty$, the parts of C that are off the real axis give a vanishing contribution to the left-hand side of (15) (because the sign of the imaginary part was chosen to make the exponent become an exponentially *decreasing* function of $|p|$), so equation (15) says that the contribution from the part of C that is on the real axis – namely (14) – must also be zero in that limit. Altogether, this shows that the remainder in equation (4) goes to zero in the continuum limit, as claimed.

8 References

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9 References in this series

Article **00980** (https://cphysics.org/article/00980):
"The Free Scalar Quantum Field: Vacuum State" (version 2022-08-23)

Article **30983** (https://cphysics.org/article/30983):
"The Free Scalar Quantum Field: Particles" (version 2022-08-23)

Article **44563** (https://cphysics.org/article/44563):
"The Free Scalar Quantum Field in Continuous Spacetime" (version 2022-09-24)

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