Positivity in Path Integrals with Scalar Fields and Gauge Fields

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Abstract In quantum field theory, models are often constructed using the path integral formulation, treating spacetime as a very fine lattice so that the math is straightforward. To ensure that time evolution is unitary in the resulting model, time evolution in the euclidean path integral construction should be positive definite. This article explains how to show that it is positive definite in a few standard families of models, including models with only unconstrained scalar fields, nonlinear sigma models whose target space is a sphere, principal chiral models, and Yang-Mills models. This article's approach differs from the usual textbook approach by using a path integral that includes an explicit initial state and that includes only one time-step. This simplifies the analysis and clarifies its relationship to the general principles of quantum theory.

Contents

1 Introduction

This article addresses a technical issue about models whose field variables are real-valued, sphere-valued, or group-valued. This includes the models constructed in article 63548, 51033, and 89053.

Constructing these models directly in the hamiltonian formulation makes their consistency with the general principles of quantum theory[1] clear by inspection, including the unitarity of time evolution. In that formulation, time remains continuous even though space is treated as a lattice, and time translations are implemented by unitary operators e^{-iHt}, where H is the hamiltonian.[2] One disadvantage of that formulation is that it obscures Lorentz symmetry. Treating space as a lattice is not the issue, because we can reasonably expect deviations from continuous space to be negligible at resolutions much coarser than the lattice scale. The issue is that the hamiltonian formulation obscures boost symmetry, so intuitively anticipating the presence of boost symmetry is difficult without checking the commutation relations of the operators that allegedly generate those symmetries. Those calculations are routine, but the outcomes are usually not easy to anticipate by inspection.

The path integral formulation makes Lorentz symmetry easier to anticipate. Spacetime is treated as a lattice, but again this shouldn't cause any perceptible deviations from Lorentz symmetry at resolutions much coarser than the lattice scale. However, in a naïve path integral formulation, time evolution may fail to be unitary, even in the continuous-time limit. Article 89053 explains how to fix this by using **Wick rotation**. Wick rotation is used to convert the original action in lorentzian spacetime to a **euclidean action**, which is then used to construct the **euclidean path integral**. After evaluating the path integral, the Wick rotation can be reversed to change the spacetime signature from euclidean back to lorentzian. For this to work, time evolution in the euclidean path integral should be positive definite.[3] This article shows that it is, for the models listed above.

[1] Article 03431

[2] Article 22871

[3] More carefully: it should be positive definite for at least one of the lattice actions that is consistent with the desired continuum limit. It doesn't need to be (and cannot be) positive definite for all of them.

2 The structure of the euclidean path integral

Article 89053 explains how Wick rotation is used to construct quantum models from euclidean path integrals. This article works exclusively with euclidean path integrals. A euclidean path integral defines a linear transformation from states to states. This transformation is a euclidean version of time evolution in the Schrödinger picture. If this transformation is positive definite, then Wick rotation converts it to a unitary transformation, as required for time evolution in quantum theory. This section reviews the euclidean version of time evolution, and then the remaining sections will show that it is positive definite.

In the path integral formulation, the euclidean version of time evolution for a single time-step[4] is given by

$$\Psi'[u'] = c \int [du]\; e^{-s[u',u]}\Psi[u], \tag{1}$$

where Ψ is the state at the initial time t, Ψ' is the state at the final time $t' = t + dt$, u is the set of field variables associated with the initial time t, and u' is the set of field variables associated with the final time t'. The value of the normalization factor $c > 0$ won't be important here, except for the fact that it is positive. The function $s[u', u]$ is the **euclidean action** for a single time-step. If the field variables were discrete, then the integral (1) would be a sum and the transformation could be expressed as matrix multiplication $\Psi' = T\Psi$. The matrix T is called the **transfer matrix**, and this name is still used for the linear transformation defined by (1) even when the field variables are continuous. The goal is to show that the transfer matrix is positive definite.

In each of the models considered in this article, the euclidean action may be written as[5,6]

$$s[u', u] = s_2[u', u] + \frac{s_1[u'] + s_1[u]}{2} \tag{2}$$

[4]Spacetime is being treated as a lattice, so time is discrete.

[5]For the models involving gauge fields, this requires using the temporal gauge (section 7).

[6]Montvay and Münster (1997), section 3.2.6 (for gauge fields)

using this notation:

- s_1 is a part of the action involving field variables at only one time,
- s_2 is the part involving products of field variables at both times.

To make the notation more compact, articles 63548, 51033, and 89053 use this version instead:

$$s[u', u] = s_2[u', u] + s_1[u]. \tag{3}$$

These two forms of the action become indistinguishable in the continuous-time limit, but they are distinct when time is discrete. The symmetric form (2) makes the transfer matrix positive definite, which is a convenient (but not strictly necessary)[7] way to ensure that time evolution becomes unitary in the continuous-time limit. If desired, the formulations in articles 63548, 51033, and 89053 could be adjusted to use the symmetric form (2), but that wouldn't change the results that matter in the continuous-time limit.

The transfer matrix is positive definite if and only if the inner product between $T\Psi$ and Ψ is a positive real number for all nonzero functions Ψ in the Hilbert space. The inner product is

$$\langle\Psi|T|\Psi\rangle = c\int [du'][du]\;\Psi^*[u']e^{-s[u',u]}\Psi[u].$$

If $s_1[u]$ is real-valued, then (2) may be used to write this as

$$\langle\Psi|T|\Psi\rangle = c\int [du'][du]\;f^*[u']e^{-s_2[u',u]}f[u] \tag{4}$$

with $f[u] \equiv e^{-s_1[u]/2}\Psi[u]$. In all the models considered here, $s_1[u]$ is a real-valued polynomial with a finite lower bound, so if Ψ is square-integrable, then so is f. In that case, the condition $\langle\Psi|T|\Psi\rangle > 0$ holds for all Ψ with $0 < \langle\Psi|\Psi\rangle < \infty$ if and only if it holds for all f with $\langle f|f\rangle > 0$ and for which the integral (4) is defined, so the remaining sections won't bother writing the s_1 terms.

[7] It obviously can't be necessary, because we can always replace a positive definite transfer matrix $T(dt)$ with a modified transfer matrix $\hat{T}(dt)$ that approaches $T(dt)$ arbitrarily quickly as $dt \to 0$.

3 The main lemma

Let $\mathcal{P}$ denote the set of all sums of products of functionals $P[u', u]$ that have the factorized form

$$P[u', u] = p^*[u']p[u]. \tag{5}$$

Any functional of the form (5) satisfies

$$\int [du'][du]\ f^*[u']P[u', u']f[u] \geq 0 \tag{6}$$

for all normalizable functionals $f[u]$, because

$$\int [du'][du]\ f^*[u']p^*[u']p[u]f[u] = \left| \int [du]\ p[u]f[u] \right|^2 .$$

Any product of such factorized functionals also satisfies (6), because such a product still factorizes as in (5). Any linear combination of such functionals with positive coefficients clearly also satisfies (6), so all elements of $\mathcal{P}$ satisfy (6). Most importantly for this article, if $P[u', u]$ is in $\mathcal{P}$, then $e^{P[u',u]}$ satisfies

$$\int [du'][du]\ f^*[u']e^{P[u',u]}f[u] > 0. \tag{7}$$

This follows from the fact that e^x may be expressed as a linear combination of powers of x with positive coefficients:

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots .$$

For each of the models considered in the remaining sections, we only need to show that $-s_2[u', u]$ is in $\mathcal{P}$, because then (7) implies that the quantity (4) is positive.

4 Positivity with unconstrained scalar fields

Article 63548 constructs a model in which the field variables are independent real variables, not subject to any constraints. In this case, the lorentzian path integral works fine: article 63548 shows that time evolution is already unitary without the help of Wick rotation. Even though it's not necessary, we can also construct those models using a euclidean path integral, and the simplicity of those models makes this a good warm-up for other models where the euclidean approach is essential.

For any given time, this family of models has a single field variable $u[\mathbf{x}]$ for each point $\mathbf{x}$ in space (treated as a lattice), and the s_2 part of the action is

$$s_2[u', u] = -2\kappa \sum_{\mathbf{x}} u'(\mathbf{x})u(\mathbf{x}) \qquad\qquad \kappa > 0.$$

The negative of this action is in $\mathcal{P}$ because it is a sum of functions of the form (5), so the general lemma (7) says that the transfer matrix is positive definite in these models, as desired.

5 Positivity with sphere-valued fields

This section considers the $O(N)$ model that is constructed in article 51033. The $O(N)$ model has N field variables at each point in the spacetime lattice. The field variables at a spatial point $\mathbf{x}$ at the initial time t will be denoted $u_j(\mathbf{x})$ with $j \in \{1, ..., N\}$, and those at a spatial point $\mathbf{x}$ at the initial time t will be denoted $u'_j(\mathbf{x})$. The title of this section says *sphere-valued* because the field variables at each point in spacetime are defined to satisfy the constraint

$$\sum_j \big(u_j(\mathbf{x})\big)^2 = 1.$$

In this model, the term s_2 in the action (2) is

$$s_2[u', u] = -2\kappa \sum_{\mathbf{x}} \sum_j u'_j(\mathbf{x}) u_j(\mathbf{x}) \qquad\qquad \kappa > 0.$$

The same reasoning as in section 4 shows again that the transfer matrix is positive definite in these models, as desired.

6 Positivity in principal chiral models

Article 51033 constructs a family of models in which the field variables take values in a unitary matrix representation ρ of a compact Lie group. Let $\bar{u}(\mathbf{x})$ denote the adjoint of the field variable $u(\mathbf{x})$. The s_2 part of the action in these models is

$$s_2[u', u] = -\kappa \sum_{\mathbf{x}} \Big(\text{trace}\big(u'(\mathbf{x})\bar{u}(\mathbf{x})\big) + \text{c.c.}\Big)$$

with $\kappa > 0$. To use the lemma (7), we only need to show that the function

$$P[u', u] \equiv \text{trace}\big(u'(\mathbf{x})\bar{u}(\mathbf{x})\big)$$

is in $\mathcal{P}$. Here's the proof:

$$\begin{aligned}\text{trace}\big(u'(\mathbf{x})\bar{u}(\mathbf{x})\big) &= \sum_{j,k} \big(u'(\mathbf{x})\big)_{kj}\big(\bar{u}(\mathbf{x})\big)_{jk} \\ &= \sum_{j,k} \big(\bar{u}'(\mathbf{x})\big)_{jk}\big(\bar{u}(\mathbf{x})\big)_{jk}.\end{aligned}$$

The first step is just the definition of the trace. The last step used the fact that the matrix representation is unitary. The last line is a sum of functions of the form (5), so lemma (7) implies that the transfer matrix is positive definite, as desired.

7 Positivity in models with gauge fields

Article 89053 constructs another family of models in which the field variables take values in a unitary matrix representation of a compact Lie group, like in section 6, but now the field variables are associated with links of the lattice instead of with sites of the lattice. The gauge-invariant form of the action involves products of four link variables (associated with the four links around the perimeter of a plaquette), but in the **temporal gauge**,[8] that part of the action reduces to

$$s_2[u', u] = -\kappa \sum_{\ell} \Big(\text{trace}\big(u'(\ell)\bar{u}(\ell)\big) + \text{c.c.}\Big)$$

with $\kappa > 0$, where the sum is over links ℓ instead of over sites $\mathbf{x}$. In this context, the link (or site) is nothing more than an index used to label the different field variables, so the proof that the transfer matrix is positive works just like it did in section 6.

[8] Articles 89053 and 00951

8 Reflection positivity

This article described a way to prove positivity of the transfer matrix in models whose lattice action has only nearest-neighbor interactions,[9] in the sense that it does not involve any products of field operators separated by more than one time-step. That's the context in which equation (1) makes sense. A more generally applicable approach is to use **reflection positivity**, which can be used in the context of a path integral without any explicitly-specified initial or final state.[10]

To define reflection positivity, consider a model defined on a d-dimensional hypercubic spacetime lattice, and let t_0 be any value of the time coordinate that may either be a time occupied by lattice sites (for **site-reflection positivity**) or a time halfway between two times occupied by lattice sites (for **link-reflection positivity**). *Reflection positivity* means that the model has an antilinear mapping Θ from functions F of the field variables at times $t > t_0$ to those at times $t < t_0$ such that the expectation value of $(\Theta F)F$ is always nonnegative.[11] Either site- or link-reflection positivity can be used to deduce the positivity of T^2, the transfer matrix for two consecutive time-steps.[12] That's sufficient for proving the existence of a Hilbert space and the existence of a Hamiltonian whose spectrum has a lower bound. If site- and link-reflection positivity both hold, then the positivity of T itself can be deduced.[13] The models considered in this article satisfy reflection positivity of both types,[14] implying that T itself is positive. That's consistent with the results derived in this article.

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[9]The word *interaction* has different meanings in quantum field theory. It often refers to any term in the action involving a product of field variables with three or more factors (higher than quadratic), but here it means any term in the action involving a product of field operators, even if it's only quadratic.

[10]Article 63548

[11]Montvay and Münster (1997), equation (4.90)

[12]The text below equation (21) in Usui (2012) says that link-reflection positivity is sufficient for this even in models whose action involves non-nearest-neighbor interactions.

[13]Montvay and Münster (1997), end of section 1.5.3 and end of section 4.2.3; Menotti and Pelissetto (1987); Usui (2012), text below equation (49)

[14]Montvay and Münster (1997), end of section 1.5.3 (for scalar fields); Montvay and Münster (1997), section 3.2.8 (for gauge fields); Menotti and Pelissetto (1987); (for gauge fields); Usui (2012), beginning of section 3.3

9 References

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