Treating Space as a Lattice

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Abstract Many introductions to quantum field theory (QFT) rely on perturbation theory – the art of using small-parameter expansions to approximate an exact expression – without ever clearly *defining* the exact expression in the first place. Everything in QFT makes more sense, both mathematically and physically, when we start with a nonperturbative definition instead. The only known nonperturbative constructions of many models involve at least temporarily replacing continuous space or spacetime with a discrete lattice. (This is clearly artificial, but that doesn't matter if the model isn't meant to be a Theory of Everything anyway.) This article introduces some basic concepts and conventions that several other articles in this series will use when defining QFTs on a spatial lattice.

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1 Introduction

We usually model space as a continuum. This mathematical idealization is consistent with all direct experimental evidence. However, in quantum field theory (QFT), the only known mathematically rigorous construction of most models involve at least temporarily treating space (or spacetime) as a discrete lattice. The definition of a derivative is a good analogy:

$$\frac{df(x)}{dx} \equiv \lim_{x' \to x} \frac{f(x') - f(x)}{x' - x}. \tag{1}$$

In this definition, the ratio must be computed using finite differences *before* taking the limit. Otherwise, the result would be nonsense:

$$\frac{\lim_{x' \to x}\Big(f(x') - f(x)\Big)}{\lim_{x' \to x}\Big(x' - x\Big)} = \frac{0}{0}.$$

The situation in QFT is similar: if we try to take the continuum limit too early in the process of calculating something, the result is undefined. We must wait until the end of the calculation to take the continuum limit, if ever.[1] In practice, taking the continuum limit is not even really necessary. Choosing the lattice scale to be much finer than the finest experimentally resolvable scale is sufficient.

A model defined on a lattice can only approximately respect translational and rotational symmetries. The deviation from exact symmetry can be negligible on a sufficiently fine lattice (article 21916), but the lattice still tends to make calculations awkward. Most of the awkwardness can be avoided in practice, because we can do most of the calculation using continuum notation and continuum techniques, resorting to the the lattice formulation only for those steps whose mathematical meaning would be truly unclear without it. This article introduces some basic notation and conventions for the simplest type of spatial lattice, emphasizing the relationships to their continuous-space cousins.

[1] Some lattice QFTs don't have nontrivial continuum limits.

2 The (hyper)cubic lattice

Let D denote the number of spatial dimensions. Continuous space can be approximated by a D-dimensional (hyper)cubic lattice. Other lattices can also be used,[2] but the (hyper)cubic lattice is intuitive and generalizes easily to any number of dimensions. For the rest of this article, the word *lattice* means (hyper)cubic lattice.

Let K denote the number of **sites** along each axis, so the total number of sites is K^D. Each site has $2D$ nearest neighbors. Let ϵ denote the **lattice spacing**, the distance between nearest neighbors. The overall linear size of the lattice will be denoted

$$L \equiv \epsilon K.$$

To approximate practically continuous space of practically infinite volume, we can use values like[3]

$$K = 10^{200\,000\,000} \qquad \epsilon = 10^{-100\,000\,000} \text{ meter} \qquad L = 10^{100\,000\,000} \text{ meters.}$$

Each site is labelled by a list $\mathbf{x} = (x_1, ..., x_D)$ of D coordinates, each of which is an integer multiple of ϵ.

The math is cleanest if we take the lattice to be **periodic**, which means that each component of $\mathbf{x}$ is defined modulo L. Then the lattice has no boundary even though it is finite: it wraps back on itself in each of the D dimensions, so each sites on one edge of the lattice has a nearest neighbor on the opposite edge. This wrapping doesn't cause any artifacts as long as we only consider applications involving regions of size $\ll L$, which may always be arranged by taking L to be sufficiently large.

An unordered pair of nearest-neighbor sites is called a **link**. A set of four nearest neighbors forming a square is called a **plaquette**. In a periodic lattice, the total number of links is $K^D \times D$, and the total number of plaquettes is $K^D \times D(D-1)/2$.

[2] We can even use a so-called **random lattice**, which isn't really a *lattice* in the usual sense of the word, but it is a way of discretizing space.

[3] Computers can't handle numbers like this, but that's irrelevant here. Here, the motive for using a lattice is to provide mathematically unambiguous nonperturbative constructions of QFTs, not to do computer calculations.

3 Integrals on the lattice

Let $\mathbf{x}$ denote a point in space, and let $f(\mathbf{x})$ be a function of $\mathbf{x}$. The lattice version of the integral over all space is

$$\int d^D x\ f(\mathbf{x}) \to \epsilon^D \sum_{\mathbf{x}} f(\mathbf{x}). \tag{2}$$

The function

$$\delta^D(\mathbf{x}' - \mathbf{x}) \equiv \begin{cases} 1/\epsilon^D & \text{if } \mathbf{x} = \mathbf{x}' \\ 0 & \text{otherwise} \end{cases} \tag{3}$$

becomes ill-defined (as an ordinary function)[4] when $\epsilon \to 0$, This situation is related to the difficulties of defining QFTs directly in continuous space. With finite ϵ, it's an ordinary function. It has the useful property

$$\epsilon^D \sum_{\mathbf{x}} \delta^D(\mathbf{x}' - \mathbf{x}) f(\mathbf{x}) = f(\mathbf{x}'),$$

whose continuous-space cousin is

$$\int d^D x\ \delta^D(\mathbf{x}' - \mathbf{x}) f(\mathbf{x}) = f(\mathbf{x}').$$

[4] It can still be defined as a **generalized function**, also called a **distribution**.

4 Gradients on the lattice

Let $\mathbf{e}_1$, $\mathbf{e}_2$, ..., $\mathbf{e}_D$ be basis vectors for the lattice, each with magnitude ϵ. Two lattice versions of the gradient will be useful:[5]

$$\nabla_k f(\mathbf{x}) \equiv \frac{f(\mathbf{x}+\mathbf{e}_k)-f(\mathbf{x})}{\epsilon} \qquad \tilde{\nabla}_k f(\mathbf{x}) \equiv \frac{f(\mathbf{x})-f(\mathbf{x}-\mathbf{e}_k)}{\epsilon}. \tag{4}$$

They both reduce to the usual gradient in the continuum limit. On a periodic lattice, they are related by this integration-by-parts identity:

$$\epsilon^D \sum_{\mathbf{x}} \Big(\nabla f(\mathbf{x})\Big) g(\mathbf{x}) = -\epsilon^D \sum_{\mathbf{x}} f(\mathbf{x}) \tilde{\nabla} g(\mathbf{x}). \tag{5}$$

Another lattice version of the gradient is

$$\frac{\nabla+\tilde{\nabla}}{2}.$$

This one goes into itself under integration-by-parts (again on a periodic lattice):

$$\epsilon^D \sum_{\mathbf{x}} \left(\frac{\nabla+\tilde{\nabla}}{2} f(\mathbf{x})\right) g(\mathbf{x}) = -\epsilon^D \sum_{\mathbf{x}} f(\mathbf{x}) \frac{\nabla+\tilde{\nabla}}{2} g(\mathbf{x}).$$

These identities are valid even if $f(\mathbf{x})$ and $g(\mathbf{x})$ are operators that don't commute with each other, as are the rest of the identities in this article.

The gradient ∇ defined by (4) satisfies this version of the product rule:

$$\nabla_k(fg) = (\nabla_k f)g + f(\nabla_k g) + \epsilon(\nabla_k f)(\nabla_k g).$$

The continuum limit deals with functions that vary only very gradually compared to the lattice scale, in which case the last term is negligible compared to the first two terms (if they're nonzero).

In infinite space, the identity $\nabla_k x^j = \delta_{kj}$ would be valid. On a finite lattice, it is valid only in the bulk of space, not at the boundaries.

[5] The components of $\mathbf{x} \pm \mathbf{e}_j$ are defined modulo L because the lattice is periodic.

5 The laplacian on the lattice

A lattice version of the laplacian ∇^2 is

$$\nabla^2 f(\mathbf{x}) \equiv \sum_k \frac{f(\mathbf{x}+\mathbf{e}_k) + f(\mathbf{x}-\mathbf{e}_k) - 2f(\mathbf{x})}{\epsilon^2}. \tag{6}$$

Use (5) to see that this satisfies

$$\epsilon^D \sum_{\mathbf{x}} \big(\nabla f(\mathbf{x})\big) \cdot \big(\nabla g(\mathbf{x})\big) = -\epsilon^D \sum_{\mathbf{x}} f(\mathbf{x}) \nabla^2 g(\mathbf{x})$$

when the gradient ∇ is defined by the first of equations (4).

6 Fourier transforms on the lattice, part 1

The discrete Fourier transform is useful for constructing eigenfunctions of the spatial translation operators. Given any function $f(\mathbf{x})$, define its Fourier transform by[6]

$$f(\mathbf{p}) \equiv \epsilon^D \sum_{\mathbf{x}} e^{-i\mathbf{p}\cdot\mathbf{x}/\hbar} f(\mathbf{x}) \tag{7}$$

where the argument $\mathbf{p}$ has D components, each of which takes values

$$\frac{2\pi\hbar}{L} \times n$$

with the integer n in the range

$$-\frac{K}{2} < n \leq \frac{K}{2}. \tag{8}$$

The quantity $\mathbf{p}\cdot\mathbf{x}/\hbar$ is always an integer multiple of $2\pi/K$. The factors of $\hbar$ are included for future convenience. The vectors $\mathbf{p}$ will be called **momentum** vectors,[7] even though they may only be indirectly related (if at all) to the conserved quantity that is also called *momentum*.

[6] In the physics literature, a function and its Fourier transform are often denoted by the same symbol with different arguments. I'm using that convention here. Remember that these are *different functions*, not just the same function evaluated at a different argument.

[7] Aside from the units-conversion factor $\hbar$, they are also called **wave vectors**, and their components are called **wavenumbers**.

7 Integrals over momenta

The lattice version of the integral over all momenta[8] is

$$\frac{1}{L^D}\sum_{\mathbf{p}}\cdots . \tag{9}$$

On a finite lattice, the sum has a finite number of terms – the same as the number of lattice sites, because of (8). If we take the continuum limit ($\epsilon \to 0$) with L fixed, then the "integral" over momenta is still a sum (9), but now with an infinite number of terms. In contrast, if we take the infinite-volume ($L \to \infty$) limit with ϵ fixed, then (9) becomes

$$\int_{\text{BZ}} \frac{d^D p}{(2\pi\hbar)^D}\ \cdots ,$$

where the subscript BZ means that the integral is restricted to the **Brillouin zone** defined by

$$|p_n| < \frac{\pi\hbar}{\epsilon}$$

for each component p_n of $\mathbf{p}$. If we take both $\epsilon \to 0$ and $L \to \infty$, then (9) becomes

$$\int \frac{d^D p}{(2\pi\hbar)^D}\ \cdots ,$$

where now the integral is over all real values of each component p_n of $\mathbf{p}$.

[8] *Momenta* is the plural form of *momentum*.

8 Fourier transforms on the lattice, part 2

As before, use the letter $\mathbf{x}$ for a quantity whose components are integer multiples of ϵ, and use the letter $\mathbf{p}$ for a quantity whose components are integer multiples of $2\pi\hbar/L$. Then these identities hold:

$$\begin{aligned} \frac{1}{L^D}\sum_{\mathbf{p}} e^{i\mathbf{p}\cdot(\mathbf{x}'-\mathbf{x})/\hbar} &= \delta(\mathbf{x}'-\mathbf{x}) \\ \epsilon^D\sum_{\mathbf{x}} e^{i(\mathbf{p}'-\mathbf{p})\cdot\mathbf{x}/\hbar} &= (2\pi\hbar)^D\delta(\mathbf{p}'-\mathbf{p}) \end{aligned} \tag{10}$$

with $\delta(\mathbf{x}'-\mathbf{x})$ defined by (3) and $\delta(\mathbf{p}'-\mathbf{p})$ defined by

$$(2\pi\hbar)^D\delta(\mathbf{p}'-\mathbf{p}) \equiv \begin{cases} L^D & \text{if } \mathbf{p}=\mathbf{p}' \\ 0 & \text{otherwise.} \end{cases} \tag{11}$$

The functions $\delta(\mathbf{x}'-\mathbf{x})$ and $\delta(\mathbf{p}'-\mathbf{p})$ are normalized differently, even though they are denoted by the same symbol. This notational compromise is used to match the standard notation when $\epsilon \to 0$ and $L \to \infty$. In particular,

$$\int d^Dx\ \delta(\mathbf{x}'-\mathbf{x}) = 1 \qquad\qquad \int \frac{d^Dp}{(2\pi\hbar)^D}\ (2\pi\hbar)^D\delta(\mathbf{p}'-\mathbf{p}) = 1.$$

Use the identities (10) to confirm that equation (7) is equivalent to the inverse relationship

$$f(\mathbf{x}) = \frac{1}{L^D}\sum_{\mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{x}/\hbar} f(\mathbf{p}). \tag{12}$$

Again, the functions $f(\mathbf{x})$ and $f(\mathbf{p})$ are distinguished from each other by the letters used for their arguments (footnote 6). This convention is especially efficient when working with several different functions and their Fourier transforms.

9 The low-momentum approximation

As before, let $f(\mathbf{p})$ denote the Fourier transform of $f(\mathbf{x})$, defined by equation (7). The fourier transform of $\nabla f(\mathbf{x})$ is $\nabla(\mathbf{p})f(\mathbf{p})$, where $\nabla(\mathbf{p})$ is the list of D functions defined by

$$\nabla_n(\mathbf{p}) \equiv \frac{\exp\big(i\mathbf{p}\cdot\mathbf{e}_n/\hbar\big)-1}{\epsilon} = \frac{\exp\big(ip_n\epsilon/\hbar\big)-1}{\epsilon}. \tag{13}$$

Similarly, the Fourier transform of $\tilde{\nabla}f(\mathbf{x})$ is $-\nabla^*(\mathbf{p})f(\mathbf{p})$, and the Fourier transform of the function $\nabla^2 f(\mathbf{x})$ defined by (6) is $-|\nabla(\mathbf{p})|^2 f(\mathbf{p})$. Use (13) to get

$$|\nabla(\mathbf{p})|^2 = \sum_n \frac{2-2\cos(p_n\epsilon/\hbar)}{\epsilon^2} = \sum_n \left(\frac{2\sin(p_n\epsilon/2\hbar)}{\epsilon}\right)^2.$$

The approximations

$$\nabla(\mathbf{p}) \approx \frac{i}{\hbar}\mathbf{p} \qquad\qquad |\nabla(\mathbf{p})|^2 \approx \frac{\mathbf{p}^2}{\hbar^2}$$

are good whenever the components p_n of $\mathbf{p}$ are restricted to the range

$$|p_n| \ll \frac{\hbar}{\epsilon}. \tag{14}$$

In practice, taking a continuum limit is not strictly necessary, as long as the lattice spacing ϵ is much less than any physically significant scale. In many cases, we may enforce this condition by restricting the theory's applications to quantities involving only small momenta, where *small* is defined by the condition (14). If larger momenta are needed, we can make the lattice spacing smaller so that this condition is still satisfied.

10 References in this series

Article **21916** (https://cphysics.org/article/21916):
"Local Observables in Quantum Field Theory" (version 2022-04-30)