The aliasing problem in lattice field theory

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Abstract

The intrinsically nonlinear nature of quantum field theory provides a fundamental complication for lattice calculations, when the physical implications of the subtleties of Fourier theory are taken into account. Even though the fundamental fields are constrained to the first Brillouin zone, Fourier theory tells us that the high-momentum components of products of these fields "bleed into" neighbouring Brillouin zones, where they "alias" (or "masquerade") as low-momentum contributions, violating the conservation of energy and momentum, and fundamentally distorting calculations. In this paper I offer a general strategy for eliminating the artefacts of aliasing in practical calculations.

1. Introduction and motivation

There is a strange relationship between the ways that engineers and theoretical physicists employ Fourier theory. Engineers generally use it for physical applications that are, from the theoretical physicist's point of view, almost trivally simple in structure: physical equations that are often linear, or, at worst, nonlinear in ways that are simple to understand, and even simpler to describe mathematically. Physicists, in contrast, analyse almost intractably complicated mathematical descriptions of physical reality, for which Fourier techniques are but one of the fundamental tools in what can be a vast mathematical toolbox of almost unbelievable sophistication and abstraction.

It is ironic, then, that the average engineer often gets a more thorough grounding in the fundamentals of Fourier theory than the average theoretical physicist. I don't know why this is so; it seems to be something of a historical accident. That the same mathematical formalism has been developed, independently, in both fields is illustrated most starkly by the fact that the fundamental theorems and constructs of Fourier theory are named after different people, depending on which faculty department is teaching it!

It is perhaps a truism that engineers can spend much more time analysing every subtlety of the physical theory they are using to describe their creations, simply because such descriptions *are* so fundamentally simple and straightforward (from the physicist's point of view, anyway). Nevertheless, it seems to me that there are some lessons that engineers have long learnt, from their extensive application of Fourier theory to real-world applications (when a simple mathematical oversight can mean the difference between a device working as

designed or failing dismally), that have not been sufficiently hammered home to theoretical physicists—if they have, indeed, been explicitly recognised as problems at all.

I believe that the most insidious of these is rooted in the simple process of forming products of fields in lattice field theory. It is a fundamental theorem of Fourier theory that forming the product of two fields in position space leads to a "convolution" of their momentum-space representations. This process axiomatically leads to the Fourier transform of the product "bleeding out" of what the physicist calls the "first Brillouin zone" (the engineer calls it "above the Nyquist frequency") into the surrounding "zones", which necessarily means that it is automatically "shifted down" in momentum. The engineer calls this phenomenon "aliasing": high-momentum components "masquerade" as low-momentum components, and generally completely destroy the fidelity of the low-frequency signal in the process. The physicist generally describes the result as being analogous to an "Umklapp process" in a crystal, because this is the physical example (with *real* lattices, no less) for which this phenomenon is most familiar.

No matter what it is called, this phenomenon can be insidiously devastating for any lattice calculation aiming to obtain as accurate a result as possible for a given amount of computing power. The fact that this phenomenon violates the conservation of energy and momentum should be sufficient to ring alarm bells for any theorist (there is no physically real "crystal" to supply the Umklapp momentum in quantum field theory—it just comes from nowhere!). That fields end up being in the wrong place in momentum space is of concern not just to the theorist, but also the pragmatist who simply wants to extract physically meaningful numbers from a lattice calculation.

A simple example will suffice to demonstrate the general havoc wreaked by aliasing. Imagine that we wish to compute some sort of expectation value, that depends on a product of some number of fundamental fields, together with a number of operators acting on the fields. Computing the expectation value corresponds to evaluating the Fourier transform of this result at zero momentum. However, if aliasing is not prevented, we find that there are *two* contributions to the result. The first is the true zero-momentum result due to the latticised approximation of the physical system (with whatever unavoidable approximations and inaccuracies that that entails), which is what we are trying to extract. The second is due to the interaction of the components of each field (and the operators in question) *at high momentum values*, which has been aliased down to zero momentum due to the fundamental properties of Fourier theory. The result, of course, comes to us as a single number, with these two contributions inextricably intertwined.

It may come as a shock, to some, that this second contribution is present at all, and is to a greater or lesser extent confounding the entire lattice calculation by its presence. Indeed, the components that make up the second contribution rightly belong at *high* momentum values—outside the first Brillouin zone completely. What are they doing back at zero momentum?

Such is the fun and games that one encounters if one entrusts Fourier theory with our calculations, without first "reading the fine print" of that mathematical formalism. In the rest of this paper, I will try to provide a "user's guide" for Fourier theory, in which this "fine print" is enlarged, and made intelligible. For many readers, much of what I will review here is like "kindergarten physics"—not worried about since undergraduate days; but when it is all put together, the importance of its ramifications for lattice calculations may be surprising. Other readers may find useful the collecting together of the fundamental theorems of Fourier

theory, and its connection with physical reality, which is often developed somewhat flippantly and "on the run" in elementary physics applications. Finally, I will offer a general strategy for removing the aliasing problem at its root, that may be of use in practical lattice calculations.

2. A review of the fundamentals of Fourier theory

In this section I provide a brief overview of the fundamental mathematical elements of Fourier theory. I concentrate on one-dimensional lattices; the extension to an arbitrary number of dimensions is elementary, and does not introduce any new constructs. The physical application and interpretation of this purely mathematical machinery will be discussed in the next section.

We start with a set of N lattice sites. We can label these sites with an integral index n that falls within a range of N successive integers. For example, we might have n running from 0 to $N-1$; but any other such range is equally possible. For definiteness, for the rest of this section we will assume that n runs from 1 to N.

We can define a function, say, f_n, that is defined on each of the N lattice sites. The N values f_n are not restricted in any way at all. They may follow some mathematical rule—and in practical applications usually will—but in principle they may be simply N numbers created at random.

We now define the *Fourier transform*, $F_b \equiv \mathcal{F}\{f_n\}$, as follows:

$$F_b \equiv \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{-2\pi i b n/N} f_n. \tag{1}$$

The values F_b represent lattice sites in "Fourier space". The index b, like n, can fall within any range of N successive integers, which need not match the range of n. For definiteness, however, for the rest of this section we will assume that b also runs from 1 to N.

The fundamental theorem of Fourier theory is that the function f_n can be retrieved from the function F_b by means of the *inverse Fourier transform*, $f_n \equiv \mathcal{F}^{-1}\{F_b\}$:

$$f_n \equiv \frac{1}{\sqrt{N}} \sum_{b=1}^{N} e^{+2\pi i b n/N} F_b, \tag{2}$$

which differs from (1) only in that n and b have been interchanged, f and F have been interchanged, and $-i$ has been replaced by $+i$ in the complex exponential. It is instructive to review the proof of the fundamental theorem, which is straightforward. We do this by evaluating the right-hand side of (2). Substituting F_b from (1), we have

$$\begin{aligned}
\frac{1}{\sqrt{N}} \sum_{b=1}^{N} e^{+2\pi i b n/N} F_b &= \frac{1}{\sqrt{N}} \sum_{b=1}^{N} e^{+2\pi i b n/N} \frac{1}{\sqrt{N}} \sum_{n'=1}^{N} e^{-2\pi i b n'/N} f_{n'} \\
&= \frac{1}{N} \sum_{b=1}^{N} \sum_{n'=1}^{N} e^{2\pi i b (n-n')/N} f_{n'} \\
&= \frac{1}{N} \sum_{n'=1}^{N} f_{n'} \sum_{b=1}^{N} e^{2\pi i b (n-n')/N},
\end{aligned} \tag{3}$$

where in the last line we have simply interchanged the order of performing the sums, which is permissible because the sums are manifestly finite. We now consider the last sum in (3),

$$\sum_{b=1}^{N} e^{2\pi i b(n-n')/N}.$$

There are two possible cases. If $n = n'$, the exponent will vanish for any value of b, and hence the complex exponential is unity for all values of b, and so we are simply summing up N copies of unity, which is just N. If $n \neq n'$, on the other hand, it is straightforward to verify that the sum vanishes by symmetry. In the case that $|n - n'|$ is coprime to N, then we are simply adding together all the N-th roots of unity, which are equally spaced around the unit circle in the Argand plane, and hence sum (vectorially) to zero. In the alternative case that $|n - n'|$ is not coprime to N, then if $g = \gcd(|n - n'|, N)$, we are simply adding together all the (N/g)-th roots of unity, a total of g times. Thus

$$\sum_{b=1}^{N} e^{2\pi i b(n-n')/N} = N\,\delta_{nn'}, \tag{4}$$

where δ_{ij} is the Kronecker delta symbol. Substituting (4) into (3) yields

$$\frac{1}{N}\sum_{n'=1}^{N} f_{n'}\,N\,\delta_{nn'} \equiv f_n,$$

hence establishing the fundamental theorem. The theorem equally provides that the F_b may be uniquely recovered from the f_n. Indeed, there is no fundamental mathematical distinction between the "original" space and "Fourier" space; they simply provide two distinct but equivalent representations of N complex quantities.

The expressions for the Fourier transformation (1) and its inverse (2) show why the indices n and b may be shifted by any arbitrary integral multiple of N without changing the mathematical results. Namely, if we replace n by $n + cN$, where c is an integer, then the complex exponential factor in (2) or (1) becomes

$$e^{\pm 2\pi i b(n+cN)/N} \equiv e^{\pm 2\pi i bn/N} e^{\pm 2\pi i bc} \equiv e^{\pm 2\pi i bn/N},$$

because $e^{\pm 2\pi i bc} \equiv 1$ if b and c are integers, as they are here. Likewise, if we replace b by $b + cN$, then the complex exponential factor in (2) or (1) becomes

$$e^{\pm 2\pi i (b+cN)n/N} \equiv e^{\pm 2\pi i bn/N} e^{\pm 2\pi i cn} \equiv e^{\pm 2\pi i bn/N}.$$

Let us now consider what happens if we form the product of two functions f_n and g_n,

$$(fg)_n \equiv f_n g_n.$$

If we take the Fourier transform of $(fg)_n$, we have, from (1),

$$\mathcal{F}\{(fg)_n\} = \frac{1}{\sqrt{N}}\sum_{n=1}^{N} e^{-2\pi i bn/N} f_n g_n.$$

If we now use (2) to write f_n and g_n in terms of their Fourier transforms F_b and G_b, this becomes

$$\begin{aligned}
&\frac{1}{\sqrt{N}}\sum_{n=1}^{N} e^{-2\pi ibn/N}\frac{1}{\sqrt{N}}\sum_{b'=1}^{N} e^{+2\pi ib'n/N}F_{b'}\frac{1}{\sqrt{N}}\sum_{b''=1}^{N} e^{+2\pi ib''n/N}G_{b''} \\
&= \frac{1}{N^{3/2}}\sum_{n=1}^{N}\sum_{b'=1}^{N}\sum_{b''=1}^{N} e^{2\pi i(b'+b''-b)n/N}F_{b'}G_{b''} \\
&= \frac{1}{N^{3/2}}\sum_{b'=1}^{N} F_{b'}\sum_{b''=1}^{N} G_{b''}\sum_{n=1}^{N} e^{2\pi i(b'+b''-b)n/N}, \qquad (5)
\end{aligned}$$

where again we can interchange the order of the sums because they are all manifestly finite. We can now use the result (4) for the final sum in (5), to obtain

$$\frac{1}{N^{3/2}}\sum_{b'=1}^{N} F_{b'}\sum_{b''=1}^{N} G_{b''}\,N\,\delta_{b'',\,b-b'} = \frac{1}{\sqrt{N}}\sum_{b'=1}^{N} F_{b'}G_{b-b'}.$$

This last bilinear operation in F_b and G_b is of such fundamental importance that it is given a special name, the *convolution* of F and G, and is denoted by a special symbol, the asterisk:

$$(F*G)_b \equiv \frac{1}{\sqrt{N}}\sum_{b'=1}^{N} F_{b'}G_{b-b'}. \qquad (6)$$

We have thus shown that the Fourier transform of a product of functions is the *convolution* of their Fourier transforms:

$$\mathcal{F}\{(fg)_n\} = (F*G)_b. \qquad (7)$$

It is straightforward to verify that the same theorem holds true for the inverse Fourier transform of a product of functions in Fourier space:

$$\mathcal{F}^{-1}\{(FG)_b\} = (f*g)_n, \qquad (8)$$

where convolution in the "original" space takes the exact same form as (6):

$$(f*g)_n \equiv \frac{1}{\sqrt{N}}\sum_{n'=1}^{N} f_{n'}g_{n-n'}. \qquad (9)$$

Now, the reader with a careful eye may have noticed that there is a slight problem with the definitions (6) and (9) of the convolution operation. We have specified, for definiteness, that the indices n and b will each take on values from 1 to N, for the purposes of this section. The indices in (6) and (9), however, take on values that clearly lie outside this range. For example, consider the computation of the $b = 2$ value in the convolution (6):

$$\begin{aligned}
(F*G)_2 &= \frac{1}{\sqrt{N}}\sum_{b'=1}^{N} F_{b'}G_{2-b'} \\
&= \frac{1}{\sqrt{N}}\Big\{F_1G_1 + F_2G_0 + F_3G_{-1} + \ldots + F_{N-1}G_{-N+3} + F_NG_{-N+2}\Big\}.
\end{aligned}$$

The index on G should run from 1 to N, like that on F; but here it is running from $-N+2$ to 1. So what happened?

The answer is that we made a rather uncritical use of the result (4) in deriving the convolution results (7) and (8). The correct generalisation of (4) is actually the following:

$$\sum_{b=1}^{N} e^{2\pi ibc/N} = \begin{cases} N & \text{if } c \equiv 0 \pmod{N}, \\ 0 & \text{if } c \not\equiv 0 \pmod{N}, \end{cases} \tag{4'}$$

where c is an integer. In the case of the identity (4), we had $c = n - n'$, so that the condition that selects the nonzero term is $n - n' \equiv 0 \pmod{N}$, namely, $n \equiv n' \pmod{N}$. But since both n and n' took on values between 1 and N, the only way that this congruence could hold was for the case of $n = n'$; hence the result (4) was, in fact, correct. For the final sum in (5), on the other hand, the correct application of (4′) yields

$$\sum_{n=1}^{N} e^{2\pi i(b'+b''-b)n/N} = \begin{cases} N & \text{if } b'' \equiv b - b' \pmod{N}, \\ 0 & \text{if } b'' \not\equiv b - b' \pmod{N}. \end{cases}$$

In other words, we should not have selected out the term for which $b'' = b - b'$ (which may, in general, fall outside the range of values taken on by indices b), but rather we should have looked for that (permissible) value of b'' that was congruent to $b - b'$ modulo N. For some values of b and b', the permissible value of b'' will simply be $b - b'$; for others, it will be $N + b - b'$. If we had chosen a different range of values for b, then other multiples of N would have to be added in order to obtain values of b'' within its allowed range.

Catering for these various cases in the mathematical definition of the convolution is a severe inconvenience, and spoils the elegance of its expression. The usual alternative is to deem that all indices n and b are, in fact, permitted to take on *any* integral values, but that it is implicitly assumed that any index arithmetic is ultimately carried out modulo N, and then shifted into the chosen range of values for indices of that type. This effectively stipulates that the lattices in n-space and b-space are to be understood to be formed into rings of N sites each.

Whilst this prescription provides a mathematical solution, its physical ramifications are both subtle and potentially devastating. Indeed, it is this "trick" that is fundamentally responsible for largely hiding the aliasing problem that has affected the fidelity of lattice calculations in the past.

3. Employing lattices for physical applications

The previous section has reviewed the fundamental elements of Fourier theory in purely mathematical terms, without reference to any physical application or interpretation of the results. We shall now review how correspondences between these mathematical constructs and physical reality are generally constructed.

The lattice of sites in the "original" n-space is usually taken to correspond to equispaced positions in position space; namely, we deem that the position x_n corresponding to the lattice site n is just

$$x_n \equiv na, \tag{10}$$

where a is the "lattice spacing", namely, the real (dimensionful) distance between adjacent lattice sites. (Recall that we are restricting our attention here to one-dimensional lattices; the generalisation to an arbitrary number of dimensions is elementary.) The lattice has a total (real) length of

$$L = Na. \tag{11}$$

The relation (2) now tells us that *any* arbitrary function f_n defined on the n sites x_n can be written as a suitable linear superposition of N complex exponential "waves". Based on our experience with quantum mechanics, we interpret each such wave as being an "eigenstate of momentum". Now, inverting (10) for n, we have

$$e^{2\pi ibn/N} = e^{2\pi ibx_n/Na}.$$

For this to be equivalent to the oscillating part of our usual definition of a plane wave eigenstate of momentum p, namely, e^{ipx} (where I shall always use units in which $\hbar = 1$), we therefore require

$$p_b \equiv \frac{2\pi}{Na} b. \tag{12}$$

In other words, the momentum value p is simply proportional to the index b. Now, since the "length" of the lattice in b-space is also N sites, the relationship (12) tells us that the "length" of the lattice in momentum space is just

$$\Lambda \equiv \frac{2\pi}{a}. \tag{13}$$

(The somewhat annoying factors of 2π in (12) and (13), that float around all Fourier expressions involving p, fundamentally arise because we have chosen our units such that $\hbar = 1$ rather than $h = 1$. Engineers essentially make the alternative choice, so that their "momentum space" variable is not complicated in this way. However, this throws an extra factor of 2π into the Fourier transform of the derivative operator, and so is inconvenient when we want to deal extensively with the formulation of differential equations, as we do in quantum field theory.)

So far, our connection of n-space to position space, and b-space to momentum space, has retained the fundamental mathematical symmetry between the two spaces that was evident in Sec. 2. However, once we start thinking about these spaces with a physical interpretation in mind, this mathematical symmetry begins to dissolve, because position space and momentum space do not enter into the laws of physics in identical ways—far from it, in fact.

Consider the situation in position space. Our fundamental laws of physics are translationally invariant, which means that no particular position x is fundamentally different than any other particular position x'. This translational invariance is not obeyed by the position-space lattice, as we have defined it so far: it has a finite length L, and hence has two "ends" which have only one neighbouring lattice site each. In this context, we willingly embrace the "ring" interpretation of the index n described in the previous section, so that position space is effectively wrapped into a ring of N lattice sites. This ensures that there are no "ends", albeit at the expense of imposing a fundamental periodicity on position space—namely, the

variable x can be defined to run from $x = -\infty$ to $x = +\infty$, but every function of x is forced to repeat identically with a periodicity of L. Our gut physical instinct tells us that, if we can make L sufficiently large for the physical system we are wishing to model, the "finite volume" artefacts of this periodicity (*i.e.*, the interactions between one "copy" of the physical system in position space and the adjacent "copies" of itself) can be made sufficiently small that they do not detract substantially from the fidelity of the mathematical model we are employing.

The situation in momentum space is completely different. Here we again have a lattice of finite "length" Λ. However, we do not have any fundamental property of "momentum translation invariance" that we wish to maintain. (The relativity of motion of Galilean or Lorentzian kinematics is somewhat more subtle than a simple translation in momentum space, and we can generally perform a transformation to the "centre of momentum" frame of reference, so that such invariance is of no practical concern anyway.) Rather, we consider the momentum "length" Λ to provide an upper limit to the momentum states that can contribute to our calculations. Indeed, since we have (in any sensible calculation) made the abovementioned transformation to a suitable "centre of momentum" frame of reference, we make use of our freedom to choose the range of b (and hence p) to ensure that momentum space is "centred" on $p = 0$; in other words, we choose to have p falling in the range $-\Lambda < p \leq +\Lambda$. In the context of quantum field theory, this "cutoff" in momentum space is actually quite convenient, regulating the formalism automatically by removing all of the higher-momentum states from our calculations.

Again, our very language here demonstrates the fundamentally different way that we view momentum space compared to position space. We accept implicitly the discussion of a "momentum state", because it is something that we are used to considering, even in undergraduate physics. Mathematically, however, a "momentum state" is actually quite a singular object. It corresponds to a function that has but a single component in momentum space. For example, if we are considering the momentum state corresponding to the momentum-space index $b = 3$, then the function in momentum space takes the form

$$F_b = A\,\delta_{b3}, \tag{14}$$

where A is some arbitrary amplitude. The reason that we accept such a function, without need for explicit comment, is that we have been long accustomed to the fact that any translationally-invariant wave equation will have eigenstates that are of precisely this form. Indeed, an engineer would equally accept a plane wave function without argument—perhaps, at worst, insisting on a real wave, such as

$$F_b = \frac{A}{2}\Big\{\delta_{b3} + \delta_{b,-3}\Big\}. \tag{15}$$

In contrast, we wouldn't generally talk about a "position state"; such a phrase would need to be explained in order to be intelligible. However, if we were to write down the position-space analogue of (14), namely,

$$F_n = A\,\delta_{n3},$$

then we would immediately recognise what is being considered: a delta-function in position space. Why the different description? Simply because such a function is *not* an eigenstate

of any naturally-occurring equation of physics that we are used to considering. Rather, it is a fairly advanced mathematical construct that is used in more abstract analyses of physical systems. The engineer likewise accepts it as such; but in this case there is no objection to its form—no insistence that it be "symmetrised" into a form similar to (15). Why not? Simply because it is in position space—"real" space—that the engineer insists on quantities being real (and indeed the physicist concurs, with the refinement that only *physically observable* quantities need actually be real in position space). Momentum space, in contrast, is an "artificial" or "mathematical" space, with which we learn to make an intellectual connection, but which is not the "real" world of our physical senses. Indeed, for a function to be real in position space, its Fourier transform needs to be *Hermitian* (not real) in momentum space, namely,

$$F_{-b} = F_b^*, \tag{16}$$

where the index $-b$ is understood to be taken modulo N and shifted into the correct range for momentum indices (although if we *have* centred the momentum index range on $p = 0$, then this caveat is not required). If we were to furthermore insist that the function in momentum space be *real*, then we would be restricting the function in position space to be an even function of x, which is not appropriate or applicable in general. Thus, the physicist and the engineer both accept, without question, that functions in momentum space will, in general, be complex-valued, even when they are describing real functions in position space.

Now, let us leave the divergence between our physical interpretation of position space and momentum space to one side, for the moment. Instead, let us focus on a more fundamental question: how do we connect the continuum spaces of the real world with the discrete spaces of the lattice world?

The simple answer is that we take the number of lattice sites, N, to infinity. However, by itself, simply taking $N \to \infty$ does not provide a definite connection with the real world. Rather, we must also specify how the lattice spacing, a, is to behave as $N \to \infty$. Now, as a general mathematical proposition, there is of course an infinite number of ways in which we can make a depend functionally on N. However, there are three particularly simple choices of $a(N)$ that allow a direct physical interpretation, and are of general importance in all practical applications of Fourier theory. I will now discuss each of these in turn, and review explicitly how the finite-lattice results of Sec. 2 are transformed into their infinite-lattice counterparts.

The simplest choice of $a(N)$ is just

$$a(N) = a = \text{constant}. \tag{17}$$

In other words, the real distance between lattice sites is kept constant; as we increase N, the extra sites simply increase the length of the lattice linearly, as shown by (11):

$$L(N) = Na, \qquad i.e., \quad L(N) \propto N. \tag{18}$$

The constant spacing a remains a part of the mathematical description in the continuum limit $N \to \infty$, and hence must correspond to some physical property of the system being modelled; in other words, a is a *physically real* quantity, rather than just a mathematical

symbol of our intermediate calculations. In practice, the prescription (17) would only be of use for systems that do, physically, have a lattice structure of periodicity a, such as a crystal.

Eq. (13) tells us that the "length" of the momentum-space lattice will be a constant, regardless of the value of N:

$$\Lambda(N) = \frac{2\pi}{a} = \text{constant}. \tag{19}$$

This implies that, as N increases, more and more momentum-space lattice sites will be packed into this fixed "length" of Λ; Eq. (12) tells us that the "spacing" in momentum space between adjacent lattice sites is

$$\delta p = \frac{2\pi}{Na}. \tag{20}$$

Hence, in the limit $N \to \infty$, momentum space will become a continuum, within the "length" $\Lambda = 2\pi/a$. This is the "first Brillouin zone" of the crystallographer.

We must now determine how the Fourier transform expressions of Sec. 2 are to be transformed in the limit $N \to \infty$. Clearly, sums in position space will continue to be sums, but now over the infinite number of lattice sites. It is usual to first change the range of n from the 1 to N of Sec. 2 to a more "symmetrical" definition, such as from the least integer $> -N/2$ to the greatest integer $\leq +N/2$, so that in the limit $N \to \infty$ the sum over n will be from $-\infty$ to $+\infty$. (The alternative would be to have an infinite lattice that possesses a single end, like a ray in geometry; this somewhat complicates the mathematical description, because instead of the continuous Fourier transform we would end up with the Laplace transform, which is not quite as convenient for our purposes.)

On the other hand, sums in momentum space will clearly be converted into integrals, over the continuum of the first Brillouin zone. We have to be careful, however, in establishing this correspondence. To illustrate why this requires extreme care, it is useful to first examine the definition of the convolution in b-space, namely, Eq. (6). The usual transition to the continuum limit entails the insertion of a factor of δp inside the sum, balanced by a compensating factor of δp outside it:

$$(F{*}G)_b = \frac{1}{\delta p\sqrt{N}} \sum_{b'} \delta p\, F_{b'} G_{b-b'} = \frac{a\sqrt{N}}{2\pi} \sum_{b'} \delta p\, F_{b'} G_{b-b'}, \tag{21}$$

where it is understood that the sum over b' is over the range of integers of the first Brillouin zone. However, if we now take the limit $N \to \infty$, we do not obtain the result we might expect:

$$\lim_{N\to\infty} \frac{a\sqrt{N}}{2\pi} \sum_{b'} \delta p\, F_{b'} G_{b-b'} = \lim_{N\to\infty} \frac{a\sqrt{N}}{2\pi} \int dp'\, F(p') G(p-p') = \infty, \tag{22}$$

where we are using (12) to relate b to p (and b' to p'), and we are assuming that the integral of $F(p')G(p-p')$ is finite. The problem is the factor of $\sqrt{N}$ outside the integral, which diverges as $N \to \infty$.

To avoid this fate, we need to redefine all functions in momentum space in the limit $N \to \infty$, by multiplying them by a multiplicative factor that is a function of N. This is

essentially an elementary application of the idea of renormalisation. Now, since $F(p)$ and $G(p)$ appear in the convolution operation symmetrically, we must apply the same renormalisation factor to each of them. However, the result of the convolution operation is itself a function in momentum space, and so should also be renormalised by the same factor. Taking these considerations into account, the divergence of (22) implies that, corresponding to any function $H(p)$ in momentum space, we should define a renormalised function

$$\overline{H}(p) \equiv H(p)\sqrt{N}, \tag{23}$$

so that

$$H(p) = \frac{\overline{H}(p)}{\sqrt{N}}. \tag{24}$$

If we insert these renormalised functions into (21), we now obtain

$$\frac{\overline{(F*G)}_b}{\sqrt{N}} = \frac{1}{\delta p\sqrt{N}} \sum_{b'} \delta p \, \frac{\overline{F}_{b'}}{\sqrt{N}} \frac{\overline{G}_{b-b'}}{\sqrt{N}},$$

so that

$$\overline{(F*G)}_b = \frac{1}{N\,\delta p} \sum_{b'} \delta p \, \overline{F}_{b'} \overline{G}_{b-b'} = \frac{a}{2\pi} \sum_{b'} \delta p \, \overline{F}_{b'} \overline{G}_{b-b'},$$

We can now take the $N \to \infty$ limit without encountering any divergence problems:

$$\overline{(F*G)}(p) = \frac{1}{\Lambda} \int_{\Lambda} dp' \, \overline{F}(p') \, \overline{G}(p-p'), \tag{25}$$

where the symbol "Λ" underneath the integral reminds us that we are integrating over a "box" of width Λ in momentum space, namely, the first Brillouin zone (regardless of how we choose its boundaries). The result (25) is the natural definition of the convolution of two continuous fields, as it corresponds to an "averaging" process, with the factor of $1/\Lambda$ balancing the integration over a box of width Λ.

We can now investigate how the inverse Fourier transform (2) relates position space and momentum space in the case of constant a as $N \to \infty$. Using the renormalised function (23) via Eq. (24), Eq. (2) gives

$$f_n = \lim_{N\to\infty} \frac{1}{\delta p\sqrt{N}} \sum_b \delta p \, e^{2\pi i b n/N} \frac{\overline{F}_b}{\sqrt{N}} = \lim_{N\to\infty} \frac{a}{2\pi} \sum_b \delta p \, e^{2\pi i b n/N} \overline{F}_b, \tag{26}$$

so that

$$f_n = \frac{1}{\Lambda} \int_{\Lambda} dp \, e^{ipx_n} \overline{F}(p). \tag{27}$$

Thus, by using the renormalised function $\overline{F}(p)$ in momentum space, we have automatically obtained a sensible result for the inverse Fourier transform. Likewise, Eq. (1) gives

$$\frac{\overline{F}_b}{\sqrt{N}} = \frac{1}{\sqrt{N}} \sum_{n>-N/2}^{\leq N/2} e^{-2\pi i b n/N} f_n, \tag{28}$$

so that the limit $N \to \infty$ is similarly well-defined:

$$\overline{F}(p) = \sum_{n=-\infty}^{\infty} e^{-ipx_n} f_n. \tag{29}$$

Finally, our use of renormalised functions in momentum space means that we need to refine the definition of the convolution operation in position space. Namely, if we form the product of two *renormalised* functions $\overline{F}(p)$ and $\overline{G}(p)$ in momentum space, then what is the corresponding operation between the functions f_n and g_n in position space? The simplest way to obtain the correct result is to directly obtain the inverse Fourier transform of $(\overline{F}\overline{G})_b$. Using (26) without the introduction of δp, together with (28), we obtain

$$\begin{aligned}
\frac{1}{N}\sum_b e^{2\pi ibn/N}\overline{F}_b\overline{G}_b &= \frac{1}{N}\sum_b e^{+2\pi ibn/N}\sum_{n'} e^{-2\pi ibn'/N} f_{n'} \sum_{n''} e^{-2\pi ibn''/N} g_{n''} \\
&= \frac{1}{N}\sum_{n'} f_{n'} \sum_{n''} g_{n''} \sum_b e^{2\pi ib(n-n'-n'')/N} \\
&= \frac{1}{N}\sum_{n'} f_{n'} \sum_{n''} g_{n''}\, N\, \delta_{n'',\, n-n'} \\
&= \sum_{n'} f_{n'}\, g_{n-n'}.
\end{aligned}$$

Thus, taking the limit $N \to \infty$, and defining

$$\mathcal{F}^{-1}\{(\overline{F}\overline{G})(p)\} \equiv (f*g)_n,$$

we find that the position-space convolution operation is also completely well-defined:

$$(f*g)_n = \sum_{n'=-\infty}^{\infty} f_{n'}\, g_{n-n'}. \tag{30}$$

So far we have examined only the case in which the $n \to \infty$ limit has been taken with the lattice spacing kept physically constant, namely, Eq. (17), which gives us an infinite lattice in position space, and a continuum limited to the first Brillouin zone in momentum space. The second simple prescription we may make for the $N \to \infty$ limit is to assume that the *length* of the position-space lattice, L, remains constant for all N:

$$L(N) = L = \text{constant}. \tag{31}$$

From (11), this implies that $a(N)$ is inversely proportional to N:

$$a(N) = \frac{L}{N}, \qquad i.e., \quad a(N) \propto \frac{1}{N}. \tag{32}$$

Eq. (13) now tells is that it is the "length" of the lattice in *momentum* space, Λ, that is proportional to N:

$$\Lambda(N) = \frac{2\pi N}{L}, \qquad i.e., \quad \Lambda(N) \propto N, \tag{33}$$

whereas it is the "spacing" in momentum space that is now a constant:

$$\delta p = \frac{2\pi}{L}. \tag{34}$$

In other words, we have the complete conjugate of the previous scenario: we have a continuum in *position* space, contained within a "box" of width L, which corresponds to an infinite lattice of states in *momentum* space. Because of the symmetry of the (finite lattice) Fourier transform, we automatically know that, in this case, we will have need to renormalise functions in *position* space:

$$\overline{h}(x) \equiv h(x)\sqrt{N}, \tag{35}$$

so that

$$h(x) = \frac{\overline{h}(x)}{\sqrt{N}}. \tag{36}$$

Now, using the fact that the spacing between lattice sites in position space is just

$$\delta x \equiv a,$$

the convolution operation in position space, (9), becomes

$$\overline{(f*g)}_n = \frac{1}{Na}\sum_{n'} a\, \overline{f}_{n'}\overline{g}_{n-n'},$$

which in the limit $N \to \infty$ gives

$$\overline{(f*g)}(x) = \frac{1}{L}\int_L dx\, \overline{f}(x')\, \overline{g}(x-x'), \tag{37}$$

where again the factor of $1/L$ naturally balances the integration over a box of width L; *i.e.*, we are computing an average over the width of the box.

Clearly, when we write the results in this way, the symmetry between position space and momentum space is manifest. This allows us to write down the constant-L analogues of (27), (29) and (30) directly:

$$F_b = \frac{1}{L}\int_L dx\, e^{-ip_b x}\overline{f}(x), \tag{38}$$

$$\overline{f}(x) = \sum_{b=-\infty}^{\infty} e^{-ip_b x} F_b, \tag{39}$$

$$(F*G)_b = \sum_{b'=-\infty}^{\infty} F_{b'}\, G_{b-b'}, \tag{40}$$

which can be confirmed by straightforward calculations.

Finally, we consider the case in which we want both position *and* momentum space to become continua in the limit $N \to \infty$. Again, there are many ways in which this can be done, but the simplest to analyse is the symmetrical prescription

$$a(N) \propto \frac{1}{\sqrt{N}}, \tag{41}$$

so that the size of the "box" in both position space and momentum space is proportional to $\sqrt{N}$:

$$L(N) \propto \sqrt{N}, \qquad\qquad \Lambda(N) \propto \sqrt{N}, \tag{42}$$

and the spacing between adjacent lattice sites in both position and momentum space is inversely proportional to $\sqrt{N}$:

$$\delta x(N) \propto \frac{1}{\sqrt{N}}, \qquad\qquad \delta p(N) \propto \frac{1}{\sqrt{N}}. \tag{43}$$

The prescription (41) requires us to fix the constant of proportionality—say,

$$a(N) = \frac{a_0}{\sqrt{N}},$$

where a_0 is some constant with the dimensions of length. However, it is practically convenient for us to choose our system of units so that $a_0 \equiv 1$, so that (42) become

$$L(N) = \sqrt{N}, \qquad\qquad \Lambda(N) = 2\pi\sqrt{N}, \tag{42$'$}$$

and (43) become

$$\delta x(N) = \frac{1}{\sqrt{N}}, \qquad\qquad \delta p(N) = \frac{2\pi}{\sqrt{N}}. \tag{43$'$}$$

If this is done, the $N \to \infty$ results can be written down directly from (1), (2), (6) and (9):

$$F(p) = \int_{-\infty}^{\infty} dx\, e^{-ipx} f(x), \tag{44}$$

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dp\, e^{ipx} F(p), \tag{45}$$

$$(F*G)(p) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dp'\, F(p')\, G(p-p'), \tag{46}$$

$$(f*g)(x) = \int_{-\infty}^{\infty} dx'\, f(x')\, g(x-x'), \tag{47}$$

with no need to "renormalise" functions in either position space or momentum space. It is an accident of pedagogical history—that should probably be rectified—that the continuum Fourier transform of Eqs. (44), (45), (46) and (47) is often taught to undergraduate students without providing a rigorous justification on the basis of it being the symmetrical $N \to \infty$ limit (41) of the discrete Fourier transform. However, with the growing importance of lattice field theory, perhaps this prejudice will slowly be overcome.

For practical lattice calculations, of course, the dependence of $a(N)$ on N does not fall neatly into any of the three simple categories listed above; indeed, one of the end-products of a lattice calculation is an estimate of a based on physically identifiable results. The $a \to 0$ and $L \to \infty$ limits are still extrapolated, but they are not both tied symmetrically to N in the way described by (41); rather, both N and the gauge coupling β are varied from calculation to calculation. This does not at all invalidate the connection made above between the lattice and continuum descriptions, but merely represents a more complicated way of taking the double limit than the simple prescription (41).

4. The problem for lattice field theory

In Sec. 2 we looked at the relationship between a discrete lattice and its Fourier transform, from a purely mathematical point of view. In Sec. 3 we began to add some physical "meat" to the description, in terms of identifying position space and momentum space, but the results were still essentially mathematical in nature. In this section we will look at where the properties of Fourier theory become problematical for lattice field theory calculations in particular.

The crux of the problem is the convolution operation. Even though we have set up our physical system to reside within a "box", in both position space and momentum space, the convolution operation goes outside this box and "reaches around the other side" of the lattice. Now, as noted above, this is not a problem in position space, because we are using the fiction of position space being wrapped into a ring (in higher dimensions, of spacetime being wrapped into an n-torus) in order to avoid having rigid boundaries that would destroy translation invariance and distort the calculations being performed inside the box. And, indeed, we find that for even the most elementary applications of a discrete space, we do wish to perform convolutions in position space; for example, the spatial derivative operator is really just a convolution, which corresponds to multiplying the function in question by ip in momentum space.

It is with convolutions in momentum space that we have trouble. This corresponds to multiplying two functions in position space, which is something that is only done for nonlinear applications—like quantum field theory. Now, we must expect that conventional Fourier transform wisdom applicable for linear applications *should* need to be augmented when we delve into the nonlinear domain; and indeed this is the case. When we multiply two fields, the high-momentum components of each field combine to "alias" (or "masqerade") as low-momentum components in the result. A simple example will suffice to demonstrate the problem. Imagine we have a field in the highest possible momentum eigenstate in the positive-x direction, namely, $p = +\pi/a$. Its spatial dependence will then be of the form $e^{i\pi x/a}$. Imagine that we now have *another* field, also in the highest possible momentum eigenstate in the positive-x direction. When we multiply the two fields in position space, the product then has a spatial dependence of simply $e^{2i\pi x/a}$, which corresponds to a momentum value of $+2\pi/a$. Indeed, in general, when we multiply in position space two fields in momentum eigenstates of p_1 and p_2, the product is in a momentum eigenstate of $p = p_1 + p_2$. When one works it through, this simply represents the principle of conservation of momentum, when quantum field theory is interpreted in terms of particles of definite momentum. However, consider the lattice representation of these two fields. For $x_n = na$, a spatial dependence

of $e^{i\pi x/a}$ simply becomes $e^{i\pi n} \equiv (-1)^n$, so that the field oscillates $+1, -1, +1, -1, \ldots$, along the position-space lattice. If we multiply this by another field having the same spatial dependence, then we end up with $+1, +1, +1, +1, \ldots$. In other words, the product of the two fields has vanishing momentum! Where did the momentum of $2\pi/a$ disappear to? It was "absorbed by the crystal in an Umklapp process"—except that in quantum field theory we have no crystal. This zero-momentum eigenstate is a purely mathematical artefact.

Another example might suffice to give a feel for the phenomenon of aliasing. Imagine that we have a field in a momentum eigenstate that is only 2/3 of the maximum momentum that can be represented on the lattice, namely, $p = 2\pi/3a$, so that it has a spatial dependence of $e^{2i\pi x/3a}$. For $x_n = na$, this is just $e^{2i\pi n/3}$, which means that its position-space dependence is

$$1, \quad -\frac{1}{2} + i\frac{\sqrt{3}}{2}, \quad -\frac{1}{2} - i\frac{\sqrt{3}}{2}, \quad 1, \quad -\frac{1}{2} + i\frac{\sqrt{3}}{2}, \quad -\frac{1}{2} - i\frac{\sqrt{3}}{2}, \quad \ldots.$$

If we multiply this field by another field that is in the same momentum eigenstate of $p = 2\pi/3a$, then we again need to simply square each of these values:

$$1, \quad -\frac{1}{2} - i\frac{\sqrt{3}}{2}, \quad -\frac{1}{2} + i\frac{\sqrt{3}}{2}, \quad 1, \quad -\frac{1}{2} - i\frac{\sqrt{3}}{2}, \quad -\frac{1}{2} + i\frac{\sqrt{3}}{2}, \quad \ldots.$$

We now recognise this to be simply $e^{-2i\pi x/3a}$; *i.e.*, the product is in a momentum eigenstate of value $p = -2\pi/3a$. In the language of quantum field theory, two particles of momentum $p = +2\pi/3a$ have combined to create a particle of momentum $p = -2\pi/3a$!

Of course, the Umklapp analogy again tells us what is happening: the two particles combined to create a momentum eigenstate of $p = +4\pi/3a$, and then the nonexistent "crystal" absorbed a momentum of $2\pi/a$ to bring the result back into the first Brillouin zone.

Let us now consider how we might repair this oversight.

5. A solution to the aliasing problem

The engineer provides a simple methodology for solving the aliasing problem: ensure that the fields are *filtered* suitably, so that there is no "cross-talk" between aliased components and genuine components in momentum space.

So how do we carry out such a programme?

The obvious "knee-jerk" reaction would be to filter every field with a low-pass filter, allowing through only momentum components $-\pi/2a < p \leq +\pi/2a$ that are no greater than *half* the maximum possible momentum (in absolute value) that can be represented on the lattice. When two such fields are multiplied together in position space, we can rest assured that the convolution process in momentum space will *not* "bleed out" of the first Brillouin zone; the sum of any two momenta can just reach the Brillouin zone boundary, but it cannot exceed it. This product of fields is then itself subjected to the same low-pass filtering, so that if we subsequently need to multiply it by some *other* (likewise filtered) field, the result again is guaranteed to be contained within the first Brillouin zone, without any aliasing artefacts.

This process ensures that aliasing is removed completely, but it has cut down the available momentum modes too harshly—it is too conservative. Consider, instead, a low-pass filter that allows through all momenta $-2\pi/3a < p \leq +2\pi/3a$ that are no greater than *two-thirds* of the maximum possible momentum value (in absolute value) that can be represented on the

lattice. If we calculate the position-space product of two fields filtered in this way, we know that the result will contain momentum values that rightly belong as high up as $p = +4\pi/3a$ and as low as $p = -4\pi/3a$. The momentum components outside the first Brillouin zone will "bleed out" and be aliased in the first zone. Those momentum components that rightly belong in the range $+\pi/a < p \leq +4\pi/3a$ will be "aliased down" by the subtraction of a "crystal momentum" of $2\pi/a$ into the range $-\pi/a < p \leq -2\pi/3a$. Likewise, those components that rightly belong in the range $-4\pi/3a < p \leq -\pi/a$ will be "aliased up" by addition of a "crystal momentum" of $2\pi/a$ into the range $+2\pi/3a < p \leq +\pi/a$. In other words, the momentum ranges $-\pi/a < p \leq -2\pi/3a$ and $+2\pi/3a < p \leq +\pi/a$ are a mess: they are a combination of the genuine components of the product, polluted by the aliased components from the other end of the spectrum.

This does not seem to be much of an advance. However, consider what we now do: we *filter the result* with the same low-pass filter, so that it is ready for any further products that we may need to form in position space. This filters out the polluted momentum ranges completely; we are left with the components in the range $-2\pi/3a < p \leq +2\pi/3a$ that represent the product with perfect fidelity! (By "perfect fidelity" I do not mean that they represent the continuum exactly, because the lattice has provided a high-momentum regulator that removes momentum modes outside this range from the outset; rather, we have a perfect representation of the *regulated* theory, within this regulated momentum range.)

In other words, the price we need to pay to remove aliasing from our lattice calculations is the complete elimination of one-third of the momentum modes in each dimension. For four-dimensional calculations, this means that we retain $(2/3)^4 = 16/81$ of the modes originally present on a lattice of any given dimensions, so that roughly four-fifths of them have been discarded (there are lots of "hypercorners" in a hypercube!).

This reduction in momentum modes might seem to be wasteful: doesn't this mean that we will need to spend five times as long performing the same lattice calculation with the same hardware? I must emphasise that nothing could be farther from the truth. The momentum modes that we are eliminating are actually *distorting* calculations that are done without their elimination. Indeed, in recent years there has been a recognition of what has been called "noise" in the high-momentum components (short-distance structure) of lattice fields, and attempts have been made to "smooth" the fields slightly, to filter out some of this "noise". However, if this "noise" *was* truly noise—uncorrelated statistical hiss—then it would not affect lattice calculations systematically at all; it would simply add to the inherent noise of the Monte Carlo process, and disappear in the mean. Aliasing, in contrast, does *not* disappear on the average: it represents a form of "wrap-around" in momentum space, that can make finite contributions systematically. Indeed, since loop diagrams in field theory inherently *diverge* for high momentum, there is the potential for aliasing artefacts to completely swamp the genuine contributions to any calculation.

6. Exact expressions for the antialiasing operator

In the previous section I argued that fields in lattice field theory calculations should be passed regularly through an "antialiasing filter" to eliminate all aliasing from the resulting calculations. The required filter is what the engineers call a "low-pass filter": it allows through momentum components in the range $-2\pi/3a < p \leq +2\pi/3a$ without distortion,

and eliminates completely all components of higher momentum (in absolute value).

The position-space form of such an operator for an infinite lattice can be derived by using the same method as was employed in [1] for the SLAC derivative operator, and the corresponding finite-lattice expressions can be derived by using the same method as was employed in [2] to "wrap" the operator around the finite lattice an infinite number of times. These are the tasks that we shall carry out in this section.

The "trick" of [1] was to start with what we described in Sec. 3 as the "constant a" limit of $N \to \infty$, namely, we consider an infinite lattice in position space with spacing a, which corresponds to a continuum in momentum space within the first Brillouin zone. Our antialiasing is then simply described by

$$F(p) = \begin{cases} 1 & \text{if } -2\pi/3a < p \le +2\pi/3a, \\ 0 & \text{otherwise.} \end{cases} \tag{48}$$

The ("renormalised") inverse Fourier transform (27) can be performed in closed form:

$$f_n^\infty = \frac{a}{2\pi} \int_{-2\pi/3a}^{+2\pi/3a} dp\, e^{ipx_n} = \frac{a}{2\pi i x_n} \Big\{ e^{+2\pi i x_n/3a} - e^{-2\pi i x_n/3a} \Big\},$$

which, from the definition of the sine function, and $x_n \equiv na$, yields

$$f_n^\infty = \frac{a \, \sin(2\pi n/3)}{\pi n}. \tag{49}$$

(The superscript of "∞" reminds us that we are working with an infinite lattice at this stage.) Let us work in "lattice units" and set $a = 1$. To calculate f_0 we need to take a limiting process for $n \to 0$, for which $\sin(2\pi n/3) \approx 2\pi n/3$, so that $f_0 = 2/3$. For all other $n \equiv 0 \pmod 3$, f_n is proportional to $\sin(2\pi k)$ where $k = n/3$, and hence f_n vanishes. For $n \equiv 1 \pmod 3$, we have $\sin(2\pi/3 + 2\pi k) \equiv \sqrt{3}/2$, so that $f_n = \sqrt{3}/2\pi n$. Likewise, for $n \equiv 2 \pmod 3$, we have $\sin(4\pi/3 + 2\pi k) \equiv -\sqrt{3}/2$, so that $f_n = -\sqrt{3}/2\pi n$. Thus, putting these together, we have

$$f_n^\infty = \begin{cases} \dfrac{2}{3} & \text{if } n = 0, \\ +\dfrac{\sqrt{3}}{2\pi n} & \text{if } n \equiv 1 \pmod 3, \\ -\dfrac{\sqrt{3}}{2\pi n} & \text{if } n \equiv 2 \pmod 3, \\ 0 & \text{if } n \equiv 0 \pmod 3 \text{ and } n \neq 0. \end{cases} \tag{50}$$

We find that f_n is an even function of n; it has a central term of $2/3$, and as we move away from $n = 0$ the terms alternate $+, -, 0, +, -, 0, \ldots$, falling off as $1/n$, with a numerical coefficient of $\sqrt{3}/2\pi$. The sum of all the terms is

$$\sum_{n=-\infty}^{\infty} f_n = \frac{2}{3} + \frac{\sqrt{3}}{\pi} \sum_{k=0}^{\infty} \Big(\frac{1}{3k+1} - \frac{1}{3k+2} \Big) = 1,$$

as expected: the filter f_n spreads a delta function out across the lattice without changing its integrated value, and so when convolved with any other function g_n will spread it out somewhat (filtering out the highest momentum states) without changing its average value.

Let us now consider obtaining closed-form expressions for f_n^N for a finite lattice of N sites. Since the general method has been described in lengthy detail in [1], I will not repeat it here, but merely cut directly to the intermediate results.

Clearly, the simplest analysis is for the case when $N \equiv 0 \pmod 3$, because the groups of three successive terms in the infinite-lattice result (50) will line up in columns. Specifically, all of the $n \equiv 0 \pmod 3$ will fall on every third site, and so f_n will vanish for all $n \equiv 0 \pmod 3$ except $n = 0$, which will retain its infinite-lattice value of $2/3$. For $n \not\equiv 0 \pmod 3$, we obtain the sum

$$f_{n \not\equiv 0 \,(\mathrm{mod}\ 3)}^{N \equiv 0 \,(\mathrm{mod}\ 3)} = \frac{1}{\pi} \sin\Bigl(\frac{2\pi n}{3}\Bigr) \sum_{k=0}^{\infty} \Bigl\{ \frac{1}{Nk+n} - \frac{1}{Nk+N-n} \Bigr\} = \frac{1}{N} \sin\Bigl(\frac{2\pi n}{3}\Bigr) \cot\Bigl(\frac{\pi n}{N}\Bigr).$$

In actual fact, this expression is also correct for $n \equiv 0 \pmod 3$, because for $n \neq 0$ the factor $\sin(2\pi n/3)$ vanishes, and the limit as $n \to 0$ is the correct value of $2/3$. Thus in full generality we may write

$$f_n^{N \equiv 0 \,(\mathrm{mod}\ 3)} = \frac{1}{N} \sin\Bigl(\frac{2\pi n}{3}\Bigr) \cot\Bigl(\frac{\pi n}{N}\Bigr), \tag{51}$$

where the limiting procedure for $n = 0$ (yielding the value $2/3$) is to be understood.

For $N \not\equiv 0 \pmod 3$, the groups of three terms "roll through" every time we loop once around the lattice. The simplest way to proceed is to make use of this $3N$-periodicity rather than the N-periodicity of the $N \equiv 0 \pmod 3$ case, and to sum up the two different sequences.

Let us start with $N \equiv 1 \pmod 3$. The $n = 0$ term picks up a correction:

$$f_{n=0}^{N \equiv 1 \,(\mathrm{mod}\ 3)} = \frac{2}{3} + \frac{\sqrt{3}}{\pi} \sum_{k=0}^{\infty} \Bigl\{ \frac{1}{3Nk+N} - \frac{1}{3Nk+2N} \Bigr\} = \frac{2}{3}\Bigl(1 + \frac{1}{2N}\Bigr). \tag{52}$$

For $n \equiv 1 \pmod 3$ we obtain

$$\begin{aligned} f_{n \equiv 1 \,(\mathrm{mod}\ 3)}^{N \equiv 1 \,(\mathrm{mod}\ 3)} &= \frac{\sqrt{3}}{2\pi} \sum_{k=0}^{\infty} \biggl\{ \Bigl(\frac{1}{3Nk+n} - \frac{1}{3Nk+3N-n} \Bigr) \\ &\qquad - \Bigl(\frac{1}{3Nk+(N+n)} - \frac{1}{3Nk+3N-(N+n)} \Bigr) \biggr\} \\ &= \frac{1}{2N\sqrt{3}} \Bigl\{ \cot\Bigl(\frac{\pi n}{3N}\Bigr) - \cot\Bigl(\frac{\pi}{3} + \frac{\pi n}{3N}\Bigr) \Bigr\}. \end{aligned}$$

For $n \equiv 2 \pmod 3$ we obtain

$$\begin{aligned} f_{n \equiv 2 \,(\mathrm{mod}\ 3)}^{N \equiv 1 \,(\mathrm{mod}\ 3)} &= \frac{\sqrt{3}}{2\pi} \sum_{k=0}^{\infty} \biggl\{ \Bigl(\frac{1}{3Nk+(2N+n)} - \frac{1}{3Nk+3N-(2N+n)} \Bigr) \\ &\qquad - \Bigl(\frac{1}{3Nk+n} - \frac{1}{3Nk+3N-n} \Bigr) \biggr\} \\ &= \frac{1}{2N\sqrt{3}} \Bigl\{ \cot\Bigl(\frac{2\pi}{3} + \frac{\pi n}{3N}\Bigr) - \cot\Bigl(\frac{\pi n}{3N}\Bigr) \Bigr\}. \end{aligned}$$

Finally, for $n \equiv 0 \pmod 3$, $n \neq 0$, we obtain

$$\begin{aligned} f_{n\equiv 0\,(\mathrm{mod}\ 3)}^{N\equiv 1\,(\mathrm{mod}\ 3)} &= \frac{\sqrt{3}}{2\pi}\sum_{k=0}^{\infty}\left\{\left(\frac{1}{3Nk+(N+n)} - \frac{1}{3Nk+3N-(N+n)}\right)\right. \\ &\qquad\left. - \left(\frac{1}{3Nk+(2N+n)} - \frac{1}{3Nk+3N-(2N+n)}\right)\right\} \\ &= \frac{1}{2N\sqrt{3}}\left\{\cot\left(\frac{\pi}{3}+\frac{\pi n}{3N}\right) - \cot\left(\frac{2\pi}{3}+\frac{\pi n}{3N}\right)\right\}, \end{aligned}$$

We can now see that there are three sequences interleaved here: one with the cot of $\pi n/3N$, one with $\pi/3$ added to the angle, and one with $2\pi/3$ added to the angle. We can thus combine them back into a single expression:

$$\begin{aligned} f_n^{N\equiv 1\,(\mathrm{mod}\ 3)} = \frac{1}{3N}\Bigg\{ &\sin\left(\frac{2\pi n}{3}\right)\cot\left(\frac{\pi n}{3N}\right) + \sin\left(\frac{2\pi}{3}+\frac{2\pi n}{3}\right)\cot\left(\frac{\pi}{3}+\frac{\pi n}{3N}\right) \\ &+ \sin\left(\frac{4\pi}{3}+\frac{2\pi n}{3}\right)\cot\left(\frac{2\pi}{3}+\frac{\pi n}{3N}\right)\Bigg\}, \end{aligned} \tag{53}$$

where again we find that the $n = 0$ term is automatically included as the $n \to 0$ limit of the generic expression.

Finally, we can carry through the same analysis for $N \equiv 2 \pmod 3$. When all the terms are recombined, the only difference from (53) is that the "rolling" factor "rolls" in the reverse direction:

$$\begin{aligned} f_n^{N\equiv 2\,(\mathrm{mod}\ 3)} = \frac{1}{3N}\Bigg\{ &\sin\left(\frac{2\pi n}{3}\right)\cot\left(\frac{\pi n}{3N}\right) + \sin\left(\frac{4\pi}{3}+\frac{2\pi n}{3}\right)\cot\left(\frac{\pi}{3}+\frac{\pi n}{3N}\right) \\ &+ \sin\left(\frac{2\pi}{3}+\frac{2\pi n}{3}\right)\cot\left(\frac{2\pi}{3}+\frac{\pi n}{3N}\right)\Bigg\}. \end{aligned} \tag{54}$$

Again, we find that the $n = 0$ term is included as the $n \to 0$ limit of the generic expression, in agreement with the first-principles result:

$$f_{n=0}^{N\equiv 2\,(\mathrm{mod}\ 3)} = \frac{2}{3} + \frac{\sqrt{3}}{\pi}\sum_{k=0}^{\infty}\left\{\frac{1}{3Nk+2N} - \frac{1}{3Nk+N}\right\} = \frac{2}{3}\left(1 - \frac{1}{2N}\right). \tag{55}$$

Finally, we can combine together the results (53) and (54) for $N \not\equiv 0 \pmod 3$, by means of a simple factor in the argument of the "rolling factor" that depends on the value of $k \equiv N \pmod 3$:

$$\begin{aligned} f_n^{N\equiv k\neq 0\,(\mathrm{mod}\ 3)} = \frac{1}{3N}\Bigg\{ &\sin\left(\frac{2\pi n}{3}\right)\cot\left(\frac{\pi n}{3N}\right) + \sin\left(\frac{2k\pi}{3}+\frac{2\pi n}{3}\right)\cot\left(\frac{\pi}{3}+\frac{\pi n}{3N}\right) \\ &+ \sin\left(\frac{4k\pi}{3}+\frac{2\pi n}{3}\right)\cot\left(\frac{2\pi}{3}+\frac{\pi n}{3N}\right)\Bigg\}. \end{aligned} \tag{56}$$

The expressions (51) and (56) are the final results of our calculation. These weights may be calculated for any value of the lattice size N, stored, and used to provide an antialiasing filter in that dimension. For a multi-dimensional lattice, we need simply perform the filtering

operation in each dimension separately. If the dimensions have different sizes, then we need to calculate and store a separate set of weights for each different size. Apart from that, however, the weights remain fixed for the entire run of the lattice calculation.

7. Stochastic implementation of the antialiasing filter

Clearly, the antialiasing filter described in the previous section is not suitable for direct implementation in practical lattice calculations. It is as horrifically nonlocal as the SLAC derivative operator studied in [1, 2, 3], linking a given site to every other site along the dimension of the lattice that we are filtering, with the absolute value of each term falling off only inversely with distance in the infinite-lattice case (with small numerical corrections for finite lattices). This means that it is not possible to truncate the series at some finite distance without severely distorting the fidelity of the operator (like we can with operators that fall off exponentially with distance)—which is precisely the fate that we want to avoid.

Thus, any practical implementation of the antialiasing filter would almost certainly employ the stochastic approach suggested in [1] for the SLAC operators. Namely, the absolute value of each weight calculated in the previous section will be taken to be the *probability* that the given linkage will be made between the site at which the antialiasing filter is being applied and the site which is at the given distance from the said site. Since the magnitude of the terms fall off inversely with distance, this implies that the average number of linkages that will be performed per site will be proportional to the *logarithm* of the length of the lattice in the given dimension, rather than being proportional to the length itself.

This is precisely the philosophy espoused in [1, 2, 3], and so does not need to be elaborated on further here. However, I need to point out one important practical error contained in those previous papers, and one improvement in the algorithm that is of particular interest to the current case.

The error relates to the requirement that each and every step of a lattice calculation maintain the unitarity of the formalism. In each of [1, 2, 3] I either stated or implied that unitarity would be maintained if every computation of a positive-distance term from a given site was always accompanied by the computation of the corresponding negative-distance term from that given site. This erroneous claim was based on a misapplication of the requirements of Hermiticity of the momentum operator. When the Hermiticity requirements are examined in closer detail, what we find is something that looks somewhat similar at a glance, but which has completely different ramifications for practical calculations, namely, that if for a Hermitian operator we perform a calculation at any site i that depends on the value of a field at any other site j, then we *must* perform the Hermitian-conjugate calculation at site j that depends on the Hermitian-conjugate value of that same field at site i. In other words, we have a form of "reciprocity requirement": if a site "gives", then it must "receive". It is *not* at all required that a positive-distance calculation from a given site be always accompanied by a negative-distance calculation from that same site (although this will be true on the average).

The algorithmic improvement relates to the implementation of the probabilistic aspect of each possible "linkage" between sites. In [1] I pointed out that the evaluation of a probability of $1/n$ (with n an integer) can be carried out much more efficiently than for an arbitrary real probability between 0 and 1, because the former can be determined directly from the

pseudo-random bitstream, without the need for floating-point calculations at all. This was very fortuitous for the considerations of [1], because the absolute value of each term of the first-derivative operator for an infinite lattice is precisely $1/n$, where n is the distance in lattice sites. This aspect of my argument remains true.

However, when in [2] I "corrected" the infinite-lattice results for finite lattices, the absolute value for the coefficient for a distance of n was changed from $1/n$ to some other number that, for small n, was very close to $1/n$. I therefore proposed that the probability for performing each calculation be maintained at $1/n$, because this yes/no decision needs to be performed as quickly as possible, as it performed for *every* distance from the given site. Rather, *if* the result of this probabilistic decision was to actually perform the linkage, then the calculation would be multiplied by a factor that was the ratio of the true (corrected) weight to $1/n$. The argument goes that, since these "correction factors" are all close to unity, the optimal balance obtained in [1] between the statistical noise of the operator and the minimisation of the number of calculations is effectively maintained, without the need to introduce floating-point calculations into the innermost probabilistic decision loop.

The logic of this argument also remains true. However, what I overlooked at the time was the fact that, as we approach the maximum possible distance from the site in question, the "correction factors" can vary substantially from unity. Of greatest practical importance is the case of the first-derivative operator for lattices with an even number of sites, because this is the situation we are usually considering for lattice field theory. In this case, the "correction factors" actually vanish as we approach the maximum distance. This means that, in an "ideal" implementation (which wouldn't care about the cost of floating-point operations), the probability of performing a calculation at large n will fall off much faster than the $1/n$ of the infinite-lattice operator. By maintaining the probability at $1/n$, we would be computing a greater number of linkages than we need to: the extra linkages would come in with a weight substantially less than unity, which means that they are wasteful of computing power when we consider the balance between statistical noise and the number of computations performed.

The solution is to slightly change the philosophy of the computation of the probabilistic weight and the correction factor. Namely, we forget about the particular structure of the SLAC derivative operator altogether, and consider the case of *any* arbitrary probability p, where $0 < p \leq 1$. We now compute $M \equiv \text{round}(1/p)$, where $\text{round}(x)$ is the closest integer to x. In the innermost lattice loop, we efficiently generate a random integer between 0 and $M-1$, as described in [1]. If this random integer vanishes, we perform the linkage calculation, and multiply it by a weight of Mp. This process then ensures that we are *always* performing a linkage that has a weight that is close to unity, and hence is maximally efficient. (The greatest deviation from unit weight occurs for high probabilities: For $p > 2/3$, we find that $M = 1$ and hence the linkage is *always* performed, with a weight that is less than unity, but no less than $2/3$. For $2/5 < p \leq 2/3$, we find that $M = 2$, so that the calculation is performed half the time, with a weight that can lie in the range $4/5 < Mp \leq 4/3$. For $p \leq 2/5$ the weight will clearly not vary from unity by more than 20%.)

Simulations of the stochastic version of the SLAC derivative operator, using this approach, have successfully demonstrated the expected behaviour. The Fourier transform of the operator has a mean value of precisely ip, with statistical noise that is distributed almost completely uniformly between all of the momentum-space components (except $p = 0$, which

vanishes by symmetry for odd N, and has a slightly larger value than the other momentum components for even N).

As a final note, the modified probabilistic algorithm described above allows us to "dial the stochasticity" of the given operator, if desired. To do this, we modify the computation of M to $M \equiv \text{round}(\eta/p)$. If the resulting M vanishes, then we set it equal to unity. If we set the dial to $\eta = 1$, we obtain the probabilistic algorithm described above. If we set the dial to $\eta = 0$, then we will always obtain $M = 1$ (pipped up from $M = 0$), and so we will always perform the linkage, which means that we have removed completely the stochastic nature of the operator. For $0 < \eta < 1$ we have an intermediate situation, in which the statistical noise is less than for $\eta = 1$, but not zero. Thus the parameter η is effectively the "stochasticity", a number that we can dial. We can even set $\eta > 1$, which will perform linkages even less often, at the expense of correspondingly increasing the weights above unity, so that the statistical noise is increased.

References

[1] J. P. Costella, `hep-lat/0207008`.
[2] J. P. Costella, `hep-lat/0207015`.
[3] J. P. Costella, `hep-lat/0404009`.