A strange property of lattices with an even number of sites

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Abstract

By examining the behaviour of the "SLAC" lattice derivative operators, it is found that lattices with an even number of sites have a somewhat strange self-consistency requirement for extra structure in the spatial derivative operator, which is not needed by lattices having an odd number of sites, and which is not at all obvious from a first-principles derivation. The general implications of this extra required structure are not, as yet, completely clear.

1. Introduction

In a previous pair of papers [1, 2] I provided a pedagogically instructive derivation of the "SLAC" spatial derivative operators of Drell, Weinstein and Yankielowicz [3, 4]. Their approach was to ensure that the Fourier transform of the spatial derivative operator takes on its ideal form in momentum space, within the first Brillouin zone—namely, that the Fourier transform of $(-i\partial/\partial x)_{\text{SLAC}}$ be identically equal to p. This is in contrast to what we obtain with $-i$ times the naïve, nearest-neighbour lattice derivative operator, which has Fourier transform of $\sin(pa)/a$ (which is only approximately linear near $p = 0$, and possesses the infamous spurious zero at the Brillouin zone boundary $p = \pm\pi/a$ that fundamentally causes the fermion doubling problem).

My goal in those earlier papers was to present a new proposal for a computationally efficient implementation of the SLAC derivative operators, by employing a stochastic philosophy. However, the pedagogical derivation of the SLAC operators, in closed form, prompted me to first check their expected fundamental properties in some practical test calculations.

Of particular interest to me were the expressions for the SLAC derivative operators for lattices with an even number of sites, because Drell, Weinstein and Yankielowicz restricted their attention to lattices with an odd number of sites only. (They furthermore did not obtain an expression for the *first*-derivative operator in closed form, in position space, even for lattices with an odd number of sites; rather, they simply represented it [4] as the inverse Fourier transform of p.) My intention was to confirm the properties of those closed-form expressions obtained in [1, 2] that were not obtained by Drell, Weinstein and Yankielowicz, to ensure that no mathematical or algebraic slips had been made in their derivation.

These confirmations were simple to obtain for the expressions for lattices with an odd number of sites. However, once the number of sites was changed to an even number, the confirmation cross-checks continually and inexplicably failed.

Although it has taken a somewhat embarrassingly long time for me to find the time to dissect the results and discover "where the wheels fell off"—and despite the fact that the source of the "problem" is blindingly obvious in retrospect—I believe that it is of sufficient intrinsic interest (and, quite possibly, fundamental importance) to those employing lattices with an even number of sites that a detailed discussion of the issue is warranted. This is the focus of the current paper.

2. The general philosophy of the previous two papers

In [1] I provided a general philosophical framework for what might be argued to be an "optimal" construction of the description of a physical system on a lattice. The basic idea is to start with the physical description that would be appropriate if both position space and momentum space are continua of infinite extent. This description then needs to be limited with a "low pass" filter in momentum space, which cuts off anything outside (what will be) the first Brillouin zone. This prepares the physical system for "sampling" onto the lattice in position space. However, *before we actually perform this sampling*, we obtain expressions for all the operators that we shall require (in our case of interest here the spatial derivative operators). Only *then* do we sample everything onto the lattice in position space.

At this stage, the physical system has been sampled onto an infinite lattice in position space, which implies an essential momentum-space description that is still a continuum, but contained within the first Brillouin zone. The second part of the process is to consider the more practically useful case when the position-space lattice is limited in extent, with periodic boundary conditions applied. This effectively "samples" the description in momentum space, as it is converted into a sequence of Dirac delta functions, which can in turn be summarised by the set of their coefficients, which effectively describes a lattice in momentum space. A one-dimensional lattice of N sites in position space then corresponds to a one-dimensional lattice of N sites in momentum space; the two descriptions are related by the discrete Fourier transform.

The difficult part of this second stage is to apply the periodic boundary conditions to the operators found in the first stage; effectively, the infinite-lattice operators have to be "wrapped around" the finite lattice an infinite number of times, with the contributions of all the "layers" to any given finite-lattice site summed up. This second stage was described in [2] for the case of the spatial derivative operators, where it was shown that the infinite sums could be performed in closed form, and indeed yield rather simple expressions.

The great advantage of this general constructional framework is that operators defined in this way in position space will automatically possess a correct (continuum) representation in momentum space—that is, at least within the first Brillouin zone and at the momentum values corresponding to the momentum-space lattice sites. In this sense they are as "optimal" as one can possibly achieve with a lattice of the given size, in that they represent their continuum counterparts with the maximum "fidelity" possible, without unnecessary distortion or artefacts. Clearly, in the case of the spatial derivative operators, the process must yield the "SLAC" operators of Drell, Weinstein and Yankielowicz, because their prescription was to simply *start* with this momentum-space fidelity, and determine the corresponding position-space operators (to the extent that they *did* actually determine these operators) by means of the inverse discrete Fourier transform.

3. Expected properties of the SLAC derivative operators

The momentum-space fidelity of the SLAC derivative operators (and by the description "SLAC" I shall henceforth refer to all of the spatial derivative operators obtained in [2] by means of what is effectively the "SLAC" philosophy, regardless of whether or not Drell, Weinstein and Yankielowicz actually obtained closed-form expressions for them in position space) means that there are a number of properties of the continuum operators that we would expect to be obeyed by their SLAC counterparts on the lattice.

Chief amongst these is the property that the second-derivative operator should be simply equivalent to two successive applications of the first-derivative operator. This can be seen most clearly in momentum space. The application of the spatial derivative operator to a function in position space is equivalent to the convolution of the said function with the "position space representation" of the spatial derivative operator (which can be obtained by applying the spatial derivative operator to the negative of the lattice representation of the Dirac delta function at the origin). By the principles of Fourier theory, a convolution in position space is equivalent to a simple multiplication in momentum space. Now, since the momentum-space representation of the SLAC first-derivative operator is simply $-ip$, applying the first-derivative operator twice is equivalent to multiplying by $(-ip)^2 \equiv -p^2$ in momentum space. But this is precisely the momentum-space representation of the SLAC *second*-derivative operator (by definition). Thus, a sequence of two successive applications of the SLAC first-derivative operator is equivalent to the application of the SLAC second-derivative operator, as is of course true in the continuum description.

This property may seem to be almost trivial, until one realises that it is *not* obeyed by the naïve first- and second-derivative operators. This is seen most quickly by remembering that the naïve first-derivative operator possesses a spurious zero at the Brillouin zone boundary (that is responsible for fermion doubling in lattice gauge theory), whereas the naïve second-derivative operator possesses no such zero [1]. Alternatively (or, really, equivalently), the period of the momentum-space representation of the naïve first-derivative operator is only half that of the naïve second-derivative operator. All that these naïve operators guarantee is that *as* $p \to 0$ the first-derivative operator approaches ip and the second-derivative operator approaches $-p^2$, so that the latter is only approximately the square of the former, as $p \to 0$; and since this relationship does not extend over all p, it means that there is no exact relationship in position space between two successive applications of the naïve first-derivative operator, and a single application of the naïve second-derivative operator.

Now, it is one thing to determine, theoretically, that two successive applications of the SLAC first-derivative operator should be equivalent to a single application of the SLAC second-derivative operator. It is quite another to verify this property, computationally, for actual lattices of various sizes. It is in this task that my own computations both succeeded and failed, as will now be described; and it is the failures that provide the phenomenon that is of fundamental interest to us.

4. Summary of the SLAC derivative operator expressions

The m-th order one-dimensional SLAC spatial derivative operator, $\Delta^{(m)}_{\mathrm{SLAC}}$, is defined by its action on an arbitrary function f_n defined on the sites $x_n \equiv na$ of a position-space lattice

containing N sites:

$$(\Delta^{(m)}_{\mathrm{SLAC}}\, f)_n \equiv \sum_{n'} {}^{(m)}c^N_{n'-n}\, f_{n'}, \tag{1}$$

where the coefficients ${}^{(m)}c^N_n$ were obtained in closed form in [1]:

$${}^{(1)}c^N_0 = 0, \tag{2a}$$

$${}^{(1)}c^{N\,\mathrm{odd}}_{n\neq 0} = \frac{(-1)^{n+1}}{na}\,\alpha\csc\alpha, \tag{2b}$$

$${}^{(1)}c^{N\,\mathrm{even}}_{n\neq 0} = \frac{(-1)^{n+1}}{na}\,\alpha\cot\alpha, \tag{2c}$$

$${}^{(2)}c^{N\,\mathrm{odd}}_0 = -\frac{\pi^2}{3a^2}\Big(1-\frac{1}{N^2}\Big), \tag{2d}$$

$${}^{(2)}c^{N\,\mathrm{even}}_0 = -\frac{\pi^2}{3a^2}\Big(1+\frac{2}{N^2}\Big), \tag{2e}$$

$${}^{(2)}c^{N\,\mathrm{odd}}_{n\neq 0} = \frac{2(-1)^{n+1}}{n^2a^2}\,\alpha^2\csc\alpha\cot\alpha, \tag{2f}$$

$${}^{(2)}c^{N\,\mathrm{even}}_{n\neq 0} = \frac{2(-1)^{n+1}}{n^2a^2}\,\alpha^2\csc^2\alpha, \tag{2g}$$

where

$$\alpha \equiv \frac{\pi n}{N}. \tag{3}$$

(The index $n'-n$ in (1) is opposite to that used for a convolution; this is notationally convenient, because it means that the value c_n is the coefficient applied in the sum to the function value at the site which is at a distance n from the site of differentiation.) The expressions (2d) and (2f) were obtained by Drell, Weinstein and Yankielowicz in [3] (where the number of lattice sites was written $2N+1$ rather than N). In the limit $N\to\infty$ we obtain the infinite-lattice expressions derived in [1]:

$${}^{(1)}c^{\infty}_0 = 0, \tag{4a}$$

$${}^{(1)}c^{\infty}_{n\neq 0} = \frac{(-1)^{n+1}}{na}, \tag{4b}$$

$${}^{(2)}c^{\infty}_0 = -\frac{\pi^2}{3a^2}, \tag{4c}$$

$${}^{(2)}c^{\infty}_{n\neq 0} = \frac{2(-1)^{n+1}}{n^2a^2}. \tag{4d}$$

5. Some example applications of the SLAC derivative operators

To appreciate the behaviour of the SLAC derivative operators it will suffice to examine just a few examples. For convenience I will here demonstrate some results for one-dimensional

lattices with a very small number of sites, as these are sufficient to set the general trend. It is straightforward to verify that the same phenomena occur for lattices with a greater number of sites.

Let us start with the case of $N = 7$. From (2a) and (2b), the first-derivative coefficients are just

$$ {}^{(1)}c_n^{N=7} = \{-0.460, +0.574, -1.034,\ 0,\ +1.034, -0.574, +0.460\}, \tag{5} $$

where the index n runs from -3 to $+3$, and where for simplicity I have set the lattice spacing to $a = 1$. (The coefficients will always be rounded off to some convenient number of significant figures.) The (discrete) Fourier transform of this operator is just

$$ {}^{(1)}C_b^{N=7} = \{-i\,1.018, -i\,0.679, -i\,0.339,\ 0,\ +i\,0.339, +i\,0.679, +i\,1.018\}, \tag{6} $$

where the momentum-space index b also runs from -3 to $+3$, where

$$ p \equiv \frac{2\pi b}{Na}. \tag{7} $$

It is clear that the Fourier transform (6) has the expected form ip, once we take account of the factor $1/\sqrt{N}$ in the definition of the (symmetrical) discrete Fourier transform, and note that

$$ \frac{2\pi}{7^{3/2}} \approx 0.339. $$

(There is a factor of $\sqrt{N}$ that floats around all discrete Fourier transform expressions, which would disappear if we more carefully considered how the lattice spacing a should vary when the number N of sites is changed, but for our current purposes I will simply insert this factor as required; it has no fundamental significance for the arguments of this paper.)

If we now convolve the operator (5) with itself—namely, apply the first-derivative operator twice—then we would expect, from the arguments given in Sec. 3, that we would obtain the second-order SLAC derivative operator. Performing this convolution numerically, we obtain

$$ \left({}^{(1)}c^{N=7} * {}^{(1)}c^{N=7}\right)_n = \{+0.00943, -0.411, +1.928, -3.223, +1.928, -0.411, +0.00943\}, \tag{8} $$

the Fourier transform of which is

$$ \left({}^{(1)}C_b^{N=7}\right)^2 = \{-2.741, -1.218, -0.305,\ 0,\ -0.305, -1.218, -2.741\}, \tag{9} $$

which can be recognised to be simply $-p^2$ by noting that

$$ \frac{(2\pi)^2}{7^{5/2}} \approx 0.305. $$

It is readily verified that the coefficients (8) are precisely those specified in expressions (2d) and (2f) for the second-order SLAC derivative, as expected.

Let us now turn to the case of $N = 8$. We immediately face a minor source of ambiguity: in the derivative coefficients, should the distances run from $n = -4$ to $n = +3$, or from

$n = -3$ to $n = +4$? The case of even N differs from that of odd N in that there is a lattice site exactly "half a lattice away" from the site at which we wish to compute the derivative, and we have to decide whether we "get to" this site means of a distance of $n = -N/2$ or of $n = +N/2$. Of course, the expression (2c) shows us that there will be no contribution from this site anyway, because for $n = \pm N/2$ we see from (3) that $\alpha = \pm\pi/2$, and the coefficient (2c) is thus proportional to $\cot(\pm\pi/2) = 0$. (When we "wrap" the operator around our finite lattice, every contribution at this "half-lattice" position for a positive value of n is cancelled out by an equal and opposite contribution from $-n$.) However, it is worth keeping this seemingly trivial annoyance in mind in what follows.

Arbitrarily choosing the lattice to run from $n = -3$ to $n = +4$, then, the coefficients specified by (2a) and (2c) for the first-derivative operation are just

$$ {}^{(1)}c_n^{N=8} = \{-0.163, +0.393, -0.948,\ 0,\ +0.948, -0.393, +0.163,\ 0\}. \tag{10} $$

Let us now immediately apply this first-derivative operator a second time. When we do so, numerically, we obtain the following coefficients:

$$ \left({}^{(1)}c^{N=8} * {}^{(1)}c^{N=8}\right)_n = \{-0.872, +0.617, +0.872, -2.159, +0.872, +0.617, -0.872, +0.925\}. \tag{11} $$

Something is obviously wrong here. The $n = 0$ coefficient is negative, as expected, and the $n = \pm 1$ coefficients are positive, again as expected, but then the $n = \pm 2$ coefficients are *also* positive, which should not occur. Indeed, the $n = \pm 3$ coefficients also have the wrong sign, as does the $n = +4$ coefficient.

Where have we gone wrong? If we use expressions (2e) and (2g) to compute the second-order derivative coefficients directly, we get a completely different set of results:

$$ {}^{(2)}c_n^{N=8} = \{+0.361, -0.617, +2.106, -3.393, +2.106, -0.617, +0.361, -0.308\}. \tag{12} $$

The most obvious explanations for this discrepancy are that either there is an error in the computational lattice machinery employed, or that an algebraic slip has caused errors in (2c), (2e) or (2g). However, it can be verified that neither of these explanations holds water.

An alternative way to check the accuracy of (2c), (2e) and (2g) is to perform the Fourier transform of each operator, because we know that the SLAC first- and second-derivative operators should have momentum-space representations of ip and $-p^2$ respectively—properties that we have verified for the case of odd N. Now, the Fourier transform of (10) is

$$ {}^{(1)}C_b^{N=8} = \{-i\,0.833, -i\,0.555, -i\,0.278,\ 0,\ +i\,0.278, +i\,0.555, +i\,0.833,\ 0\}, \tag{13} $$

which is recognised to be ip, as expected, when we note that

$$ \frac{2\pi}{8^{3/2}} \approx 0.278. $$

Likewise, when we take the Fourier transform of the coefficients (11), we obtain

$$ \left({}^{(1)}C_b^{N=8}\right)^2 = \{-1.963, -0.872, -0.218,\ 0,\ -0.218, -0.872, -1.963,\ 0\}, \tag{14} $$

which is again recognised to be of the expected form $-p^2$ when we note that

$$\frac{(2\pi)^2}{8^{5/2}} \approx 0.218.$$

This confirms that the expressions (2c), (2e) and (2g) are correct, that the convolution is being performed correctly, and that the Fourier transform engine is also operating correctly.

So why do the coefficients (11) look nothing at all like the expected coefficients (12)?

6. Why do even lattices give us a problem?

To find out why the even-lattice operators aren't behaving as expected, we need simply take the Fourier transform of the SLAC second-derivative coefficients (12):

$$^{(2)}C_b^{N=8} = \{-1.963, -0.872, -0.218,\ 0,\ -0.218, -0.872, -1.963, -3.489\}. \tag{15}$$

At first glance, this appears to be identical to the Fourier transform (14) of the result of the first-derivative operator being applied twice—but there is a crucial difference: the $b = +4$ value is -3.489 in (15), whereas it *vanishes* in (14).

What is going on here? The $b = +4$ lattice site in momentum space is, from Eq. (7), simply the site corresponding to the momentum value $p = +\pi/a$, namely, the very boundary of the first Brillouin zone. Now, *should* the second-derivative operator take a value corresponding to $-p^2$ at this boundary site, or should it vanish? Obviously, we would prefer it to take its correct (continuum) value of $-p^2$ if at all possible; and that is what has been built into the SLAC second-derivative operator, which has yielded precisely this desired value in (15). So where is the problem?

The problem is not with the second-derivative operator at all, but rather with our attempt to apply the first-derivative operator twice. Applying a derivative operator twice (*i.e.*, effectively convolving the operator with itself) is equivalent to squaring its momentum-space representation. And so, indeed, the momentum-space coefficients (14) are just the squares of the corresponding coefficients (13) (when a factor of $\sqrt{N} = \sqrt{8}$ is taken into account).

The problem, however, arises because of the momentum-space lattice site at the Brillouin zone boundary, namely, $b = +4$. Recall our earlier discussion of the ambiguity arising from the need to decide whether the "half-lattice distance" in position space should be designated $n = +4$ or $n = -4$? Here we have the completely analogous ambiguity of needing to decide whether the Brillouin zone boundary should be represented in momentum space by $b = +4$ or $b = -4$. For the SLAC *second*-derivative operator, this choice is of no fundamental import, because its Fourier transform, namely, $-p^2$, is an even function of p (and hence b); in other words, $(+4)^2$ and $(-4)^2$ will both give us the same value for the $b = \pm 4$ site. Indeed, if we were to arbitrarily choose to put the Brillouin zone boundary site at $b = -4$ in our Fourier transform engine, the Fourier transform of the SLAC second-derivative operator (12) simply becomes

$$^{(2)}C_b^{N=8} = \{-3.489, -1.963, -0.872, -0.218,\ 0,\ -0.218, -0.872, -1.963\}. \tag{16}$$

The discrepancy between (15) and (14) tells us that it is the "missing" value at $b = +4$ in (14) that is responsible for us not obtaining the expected result when we applied the SLAC

first-derivative operator twice. In isolation, this seems reasonable enough: we simply need to make sure that the "missing" value is put back in. But things start to get rather strange when we investigate the ramifications of this requirement. Presumably, we must "repair" the *first*-derivative operator, to ensure that, when we apply it twice (and hence square its representation in momentum space), the "missing" value is restored. This immediately draws our attention to the final coefficient in (13), which currently vanishes. The fundamental reason that it *must* vanish is not difficult to appreciate: the momentum eigenstate at the Brillouin zone boundary oscillates in position space at the maximum possible (Nyquist) frequency, $+1, -1, +1, -1, \ldots$, which is an even function of n. Now, the SLAC first-derivative operator is an odd function of n, and furthermore vanishes at $n = +N/2$ (or $n = -N/2$ if that had been our arbitrary choice), so no matter which position we "place" it next to the maximum-frequency eigenstate, in the convolution, it will necessarily yield a vanishing sum. For example, with $N = 8$, the operator (10) will lead to a convolution of the form

$$-0.163 - 0.393 - 0.948 + 0 + 0.948 + 0.393 + 0.163 + 0 = 0,$$

or its negative, for all positions. This symmetry argument, in fact, proves the following general theorem: *Any position-space operator that is an odd function of n, and vanishes at $n = \pm N/2$, will lead to a zero at the Brillouin zone boundary for a lattice with an even number of sites*. (This is, of course, also true for the naïve first-derivative operator [1], although in that particular case the restricted nature of this theorem—namely, that the necessary vanishing of the Fourier transform is restricted to the single site that lies on the Brillouin zone boundary—is somewhat hidden by the fact that the Fourier transform of the naïve operator approaches this zero smoothly, rather than abruptly as is the case here.)

Why does this theorem only hold for lattices with an even number of sites? Simply because lattices with an odd number of sites do not possess a momentum eigenstate that is on the Brillouin zone boundary. Not only is this obvious from the relation (7)—namely, for $p = \pm\pi/a$ we require $b = N/2$, which is only possible if N is even—but it is also clear in position space, because such an eigenstate, oscillating $+1, -1, +1, -1, \ldots$, necessarily requires an even number of sites in which to fit an integral number of $+1, -1$ pairs; otherwise, the periodic boundary conditions of the lattice would not be satisfied (*i.e.*, viewed as a ring, there would be either two $+1$ or two -1 sites next to each other). As should be clear from the above example, the general theorem applies *only* to the single momentum site at the Brillouin zone boundary, so if this site does not exist (as is the case for odd N), the theorem likewise fails to exist.

This general problem may, in fact, have been the reason why Drell, Weinstein and Yankielowicz restricted their attention exclusively to lattices with an odd number of sites—namely, to avoid the conundrum that we are now facing while trying to apply the first- and second-order SLAC derivative operators. (However, I have no direct evidence that this was their motivation for this restriction.)

7. Solving the even-lattice conundrum

It is all well and good to understand why our even-lattice operators do not have the properties we expect of them, but our ultimate goal must be to "repair" the first-derivative operator so that we can recover these properties.

Clearly, we must ensure that the second-derivative operator possesses its correct (continuum) value $-p^2$ at the Brillouin zone boundary, as we have found is explicitly obtained if we use the SLAC second-order derivative coefficients derived in [2]. To maintain the self-consistency of differential calculus on such lattices, we wish to further ensure that two successive applications of the first-derivative operator be identically equivalent to a single application of the second-derivative operator; if we didn't insist on reinstating this property, there would be little point in using the SLAC operators at all—we may as well go back to using the naïve operators, which do not obey this property except in the limit of small p.

Since a double application of the first-derivative operator is equivalent to squaring its representation in momentum space, our task must be to somehow replace the vanishing final coefficient of (13) with its correct (continuum) value of ip. In the case of (13) (taking into account the factor of $2\pi/\sqrt{8}$), we need to modify the momentum-space representation to

$$^{(1)}C_b^{N=8} = \{-i\,0.833, -i\,0.555, -i\,0.278,\ 0,\ +i\,0.278, +i\,0.555, +i\,0.833, +i\,1.111\}. \tag{17}$$

More precisely (and taking more careful note, now, of factors of a and $\sqrt{N}$), we wish to add an extra value of $+i\pi/a\sqrt{N}$ at the momentum value $p = +\pi/a$. Taking into account the factor of $1/\sqrt{N}$ in the discrete Fourier transform, this means that we wish to add to the SLAC first-derivative operator an *extra* function in position space, of the form

$$^{(2)}c_{\text{extra}}^{N\text{ even}} = \frac{i\pi}{Na}(-1)^n. \tag{18}$$

In other words, for our example of $N = 8$, we wish to change the first-derivative operator from the coefficients listed in (10) to

$$\begin{aligned} ^{(1)}c_b^{N=8} = \{\ &-0.163 - i\,0.393,\ \ +0.393 + i\,0.393,\ \ -0.948 - i\,0.393,\ \ \ 0 + i\,0.393, \\ &+ 0.948 - i\,0.393,\ \ -0.393 + i\,0.393,\ \ +0.163 - i\,0.393,\ \ \ 0 + i\,0.393\ \}, \end{aligned} \tag{19}$$

where

$$\frac{\pi}{8} \approx 0.393.$$

Clearly, the extra contribution (18) to (19), being an even function of n, avoids the consequences of the general theorem above, as it must by the way it has been constructed. And, sure enough, if we apply the operator (19) twice, we obtain precisely the SLAC second-derivative coefficients (12), as expected.

But what sort of a monster have we created?

There are a number of important objections that one may wish to make at this point. Most seriously, we made a completely arbitrary choice, when we first considered the Fourier transform to momentum space, to place the Brillouin zone boundary site at $b = +4$. What if we had, instead, chosen to put it at $b = -4$? In the case of the second-derivative operator, such a change makes nothing but a notational difference, because the Fourier transform of the second-derivative operator is an even function of b. In the case of the first-derivative, on the other hand, we must surely insist that the extra site take on its correct (continuum) value, namely, $-i\,1.111$, which is the negative of that added to (17), so that the momentum-space representation becomes

$$^{(1)}C_b^{N=8} = \{-i\,1.111, -i\,0.833, -i\,0.555, -i\,0.278,\ 0,\ +i\,0.278, +i\,0.555, +i\,0.833\}. \tag{20}$$

Now, since the position-space representation of a term at the Brillouin zone boundary is unchanged, regardless of whether we write it as $b = +4$ or $b = -4$, because

$$e^{+i\pi n} \equiv (-1)^n \equiv e^{-i\pi n},$$

this change of sign for the extra momentum-space term implies that the extra function added in position space will likewise change in sign:

$${}^{(2)}c^{N\,\mathrm{even}}_{\mathrm{extra}} = \frac{i\pi}{Na}(-1)^{n+1}, \tag{21}$$

which for our example of $N = 8$ yields

$$\begin{aligned} {}^{(1)}c_b^{N=8} = \{\ & 0 - i\,0.393,\ -0.163 + i\,0.393,\ +0.393 - i\,0.393,\ -0.948 + i\,0.393, \\ & 0 - i\,0.393,\ +0.948 + i\,0.393,\ -0.393 - i\,0.393,\ +0.163 + i\,0.393\}. \end{aligned} \tag{22}$$

Again, if we apply this operator twice, we obtain the expected analogue of (12) with a site at $n = -4$ rather than $n = +4$:

$$\left({}^{(1)}c^{N=8} * {}^{(1)}c^{N=8}\right)_n = \{-0.308, +0.361, -0.617, +2.106, -3.393, +2.106, -0.617, +0.361\}. \tag{23}$$

In other words, we can add in *either* of the extra functions (18) *or* (21)—fundamentally depending only on which end of the momentum-space lattice we choose to put the Brillouin zone boundary term—and, either way, we still get the right answers:

$${}^{(2)}c^{N\,\mathrm{even}}_{\mathrm{extra}} = \pm\frac{i\pi}{Na}(-1)^n. \tag{24}$$

So which function is "correct"? Which sign is the "right" sign: the positive or the negative?

8. "Spontaneous symmetry breaking" for even lattices

The simple answer to the question of which sign is "correct" in (24) is that they are *both* "correct". When we create a lattice with an even number of sites, we must decide whether the "half-lattice" distance in position space is to be located at $n = +N/2$ or $n = -N/2$, and we must likewise decided whether the Brillouin zone boundary site in momentum space is to be located at $b = +N/2$ or $b = -N/2$. It is the latter choice that determines whether the extra term required in the SLAC first-derivative operator should come in with the plus sign or the minus sign in (24).

Although it does not have the same physical and dynamical connotations, this situation is—mathematically, at least—completely analogous to the situation of spontaneous symmetry breaking in field theories. Here, the SLAC first-derivative operator is a real, odd function of the position-space distance n, for the case of an infinite lattice, which implies that its momentum-space representation is a purely imaginary, odd function of p. When we "wrapped" this infinite-lattice operator around a finite lattice, in [2], these properties were maintained. The consequence, however, was the introduction of a spurious zero into its momentum-space representation, at the Brillouin zone boundary. The fundamental problem is that a lattice with an even number of sites will always have a momentum eigenstate

that is "unpaired"; in other words, an even lattice by necessity breaks the symmetry in momentum space between positive and negative momenta. Now, if we do not introduce the extra function (24) into the first-derivative operator, we are effectively imposing the odd, imaginary property in momentum space on the operator by treating the site at the Brillouin zone boundary as being *both* $p = +\pi/a$ *and* $p = -\pi/a$; and since, to be an odd function of p, these sites should have equal and opposite values, we are effectively "averaging" them out to give zero. Put differently, the only way for an imaginary number to be its own negative is for the number to be zero.

The example of spontaneous symmetry breaking in field theory guides us in the current case. In field theory, we do not impose the underlying symmetry on the states of the broken-symmetry formalism; rather, we recognise that the symmetry has, indeed, been broken, and we embrace and analyse the ramifications of the symmetry being broken—understanding that for every arbitrary choice of manner of breaking of the fundamental symmetry, there will be a physically equivalent description (or an infinite number of such descriptions, for a continuous symmetry) with a different arbitrary choice of manner of breaking. Analogously, for an even lattice, we can choose to put the Brillouin zone boundary site at *either* $b = +N/2$ or $b = -N/2$, in the full knowledge that this choice is arbitrary, but that *it must be made for any definite application of the lattice for practical purposes*.

This is, admittedly, a somewhat "philosophical" justification for why the extra function (24) *should* be added to the SLAC first-derivative operator—in other words, that its omission would arguably lead to a greater divergence from the continuum reality than its inclusion. The "proof of the pudding", of course, will be the application of this prescription to real-world calculations. However, as these will take time to implement, it is worth discussing here some of the more fundamental properties of the modified first-derivative operator in general terms, so that we know what we might expect when it is used in practice.

9. Properties of the modified SLAC first-derivative operator

Earlier I argued that the most serious objection to the modification to the SLAC first-derivative operator must be the arbitrariness of the choice of sign in (24). Almost equally objectionable, however, must be the *form* of the additional function (24). The derivative operator is, naturally, a real operator in position space (as it must be, because the process of differentiation is something that can be applied to real functions, not just complex functions). The additional function (24), in contrast, is purely imaginary. Won't this destroy some fundamental property of calculus? Won't it mess up the unitarity of any quantum calculation?

It is the unitarity of the formalism that is of most concern to us here. As reviewed in [1], the only reason that the naïve first-derivative operator possesses a spurious zero at the Brillouin zone boundary—leading, fundamentally, to the fermion doubling problem—is that unitarity prevents us from computing a first-derivative on the basis of adjacent lattice sites. And, indeed, unitarity is such an important property of any quantum calculation that it would be difficult to proceed with confidence at all if it were broken—regardless of whether or not it would be restored in the continuum limit.

So let us determine whether the extra function (24) will cause us any problems with unitarity. The way to check this is to examine the momentum operator p in position space,

namely, $-i$ times the derivative operator. When we write this operator as a matrix (with columns representing the "input" function, and rows the "output" function, namely, the derivative of the original function), we require it to be Hermitian [1]. Now, (24) yields

$$p^{N\,\mathrm{even}}_{\mathrm{extra}} \equiv -i\,{}^{(2)}c^{N\,\mathrm{even}}_{\mathrm{extra}} = \pm\frac{\pi}{Na}(-1)^n. \tag{25}$$

This represents a matrix operator of the form

$$p^{N\,\mathrm{even}}_{\mathrm{extra}} = \pm\frac{\pi}{Na}\begin{pmatrix} +1 & -1 & +1 & -1 & +1 & \cdots \\ -1 & +1 & -1 & +1 & -1 & \cdots \\ +1 & -1 & +1 & -1 & +1 & \cdots \\ -1 & +1 & -1 & +1 & -1 & \cdots \\ +1 & -1 & +1 & -1 & +1 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \tag{26}$$

Although rather unfamiliar as an operator in everyday calculations, this matrix most surely is Hermitian. Thus, we cannot object to the extra function (24) on the grounds of unitarity: its inclusion will not affect the unitarity of our calculations in the least.

Of course, if we were looking to use an even lattice to perform some sort of calculation of strictly real functions (such as for an Engineering application, say), then we would still be able to object to (24) on the grounds that it would introduce "spurious" imaginary components into the calculations. On the other hand, *any* calculation on a lattice is somewhat artificial and mathematical anyway—and if the introduction of imaginary components is the price one has to pay to ensure that the self-consistency of differential calculus is maintained, on such a lattice, then it is arguable that such an introduction should indeed be made, regardless of the nature of the application.

However, it is worth examining how large in magnitude the extra terms (24) in the differential operator will actually be, relative to the "normal" terms (2c). Apart from a numerical factor of π, the magnitude of each extra term (24) is a factor of n/N smaller than the corresponding term in (2c). Thus, the "extra" terms are of roughly the same size as the "normal" terms at the farthest distances on the periodic lattice.

What does this mean? Remember that, in principle, we are actually trying to take a spatial derivative of a function *locally*, namely, that the derivative function at any position x should only depend on that part of the original function that is "local" to x. The SLAC derivative operators appear to violate this wish, because the derivative at any lattice site n depends on the value of the original function at *all* sites on the lattice. However, as emphasised in [1], this "non-locality" is an illusion, because as the number of sites N is increased, the lattice spacing is decreased, so that the contribution to the SLAC derivative operator from any finite (real) distance away from the point of differentiation vanishes as N is increased. Likewise, as N is increased, the relative contribution of the extra function (24) is decreased, and in the limit $N \to \infty$ it vanishes.

A further property of the modified derivative operator is obvious from the way we have constructed it, namely, that the only zero in its momentum-space representation is at $p = 0$; we have eliminated the spurious zero at the Brillouin zone boundary. Again, this simply restores us to the situation we already have for the case of odd N, namely, that there is no

spurious zero to start with for odd N, because there is no momentum-space lattice site on the Brillouin zone boundary. One would expect that this "momentum space fidelity" will ensure that there is no problem with fermion doubling in lattice field theory, as there is for the naïve first-derivative operator.

10. Conclusions

In this paper I have tried to show why lattices with an even number of sites contain potential pitfalls for the unwary. I have illustrated this with the example of my own blundering attempts to correctly define and implement the SLAC derivative operators on simple one-dimensional lattices. However, the fundamental principle—and warning—is, I believe, a general one; similar subtleties should apply to other aspects of field theory formulated on even lattices. The fundamental reason for this, I believe, is that such lattices break the symmetry between positive and negative momentum values that holds for any continuum formalism (and which is retained for odd lattices); a faithful representation on an even lattice requires us to "spontaneously break" this symmetry in favour of an extra momentum eigenstate at the Brillouin zone boundary of either $p = +\pi/a$ or $p = -\pi/a$, but not both.

Given the computational convenience of employing lattices with an even number of sites (generally a power of two in each dimension), the full exploration of these subtleties may prove to be of interest to practitioners in the field of lattice calculations. I will be continuing these investigations in due course, but at present the full potential ramifications are not clear to me.

Acknowledgments

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