A new proposal for the fermion doubling problem II. Improving the operators for finite lattices

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Abstract

In a previous paper I showed how the ideal SLAC derivative and second-derivative operators for an infinite lattice can be obtained in simple closed form in position space, and implemented very efficiently in a stochastic fashion for practical calculations on finite lattices. In this second paper I show how the small (order $1/N$) errors introduced by truncating the operators to a finite lattice may be removed by a small adjustment of coefficients, without incurring any additional computational cost. The derivation of these results is again presented in a simple, pedagogical fashion.

1. Truncating the SLAC derivative operators to fit on a finite lattice

In a previous paper [1] we looked at the ideal "SLAC" specification of Drell, Weinstein and Yankielowicz [2] for the spatial derivative operator on an infinite one-dimensional lattice, which demands that $-i$ times the Fourier transform of the derivative operator take on its ideal functional form,

$$p_{\text{ideal}} = p,$$

within the first Brillouin zone. Such an operator avoids the pathologies of the fermion doubling problem or the violation of chiral invariance that have plagued other sub-optimal definitions of the derivative operator, but has a representation in position space that is very "nonlocal",

$$\begin{aligned}\mathit{\Delta}_{\text{ideal}} f(x) = \frac{1}{a}\Big\{ \ldots - \frac{1}{4}f(x+4a) + \frac{1}{3}f(x+3a) - \frac{1}{2}f(x+2a) \\ + f(x+a) - f(x-a) \\ + \frac{1}{2}f(x-2a) - \frac{1}{3}f(x-3a) + \frac{1}{4}f(x-4a) - \ldots \Big\},\end{aligned} \tag{1}$$

and indeed links the lattice site at which we wish to take the derivative to every other site in the (one-dimensional) lattice. This has, historically, presented a barrier to the practical implementation of the SLAC operator in any large-scale lattice calculations.

In [1] I proposed a solution to this computational barrier, namely, that the SLAC derivative operator can be implemented in a *stochastic* fashion, so that for a one-dimensional finite lattice of N sites the average number of computations required to implement each derivative operation is of order $\log N$ rather than of order N.

However, even though the use of the ideal SLAC specification ensures that the representation (1) of the derivative operator is the best that can possibly be done for a given finite lattice spacing distance a, the "truncation" of the operation to "fit" on a lattice with a finite number N of sites in [1] introduces small errors (of order $1/N$) that detract from the "optimality" of the operator. It is desirable to remove these errors, to ensure that the stochastic SLAC derivative operator for a *finite* lattice is "optimal"—namely, the best that can possible be done.

It is first worth seeing explicitly how the "truncation" operation detracts from the fidelity of the ideal SLAC derivative operator. Let us take a truly extreme example—a lattice of only one site!—and let us assume that the underlying continuum formalism specifies that we take the *second*-derivative of some function $f(x)$. A simple derivation in [1] showed how one can obtain from first principles the expression first found by Drell, Weinstein and Yankielowicz [2] for the ideal SLAC second-derivative operation in position space, for the case of an infinite lattice:

$$\begin{aligned}\Delta^{(2)}_{\text{ideal}} f(x) = \frac{2}{a^2}\Big\{ \dots - \frac{1}{16} f(x+4a) + \frac{1}{9} f(x+3a) - \frac{1}{4} f(x+2a) \\ + f(x+a) - \frac{\pi^2}{6} f(x) + f(x-a) \\ - \frac{1}{4} f(x-2a) + \frac{1}{9} f(x-3a) - \frac{1}{16} f(x-4a) + \dots \Big\}.\end{aligned} \tag{2}$$

What happens when we "truncate" this operation to apply to the extreme case of a lattice with just one site? Clearly, we will be left with only the middle term, namely,

$$\Delta^{(2)}_{\text{truncated}} f(x)\Big|_{x=0} = -\frac{\pi^2}{3a^2} f(0). \tag{3}$$

Assuming $f(0) \neq 0$, we have somehow estimated the second-derivative of a function evaluated at just one point in space to be some nonzero value! Of course, I said above that the errors in truncating the operator are of order $1/N$; and here $N = 1$, so the errors are of order unity; in other words, the value itself has absolutely no reliability at all. But is this the best we can do?

I believe that it is not. When we restrict any physical formalism to a finite "box", we generally assume that the physical functions of relevance shall have periodic boundary conditions applied to them. (Indeed, it would be difficult to formulate a tractable analysis of most systems in momentum space if this stipulation were not to be made.) This is equivalent to thinking of a system of infinite spatial extent, made up of "boxes" stacked side-by-side along the x-axis, with the extra proviso that the contents of each box are to be considered to be identically equivalent to that of the "central box". If this is the case, then in the extreme case of a lattice with only one site, we are effectively stipulating that the value of any function at every site of the imagined infinite lattice (one such site in each of these identical "boxes") must be identical to the value of the function in the "central box" (centred on $x = 0$). In other words, the function is effectively a constant on all of the (infinite number of) lattice sites:

$$f(x_n \equiv na) = f(0) = \text{constant}.$$

In this context, our obtaining a nonzero estimate of the second-derivative in (3) looks very poor: surely, the second-derivative of a constant function is just zero!

2. Applying periodic boundary conditions to the SLAC derivative operators

The reason that the result (3) obtained above is so poor is simply because we have (by assumption) applied periodic boundary conditions to the function defined on the single lattice site, but *we have not applied periodic boundary conditions to the SLAC derivative operator*; rather, we simply "truncated" it when we had gone once around the lattice (in this case, after evaluating it at just the single lattice point). Now, the SLAC second-derivative operator (2) links the site in question to every other site on an infinite lattice. Applying periodic boundary conditions to it implies that we must go around and around the lattice an infinite number of times, calculating all of these infinite number of terms that contribute to the sum.

Performing an infinite number of calculations does not sound very palatable, from a computational point of view. However, by the very assumption of periodic boundary conditions, the function $f(x)$ itself is identically the same every time we "go past" it, and so it effectively factorises out of the sum, namely,

$$\Delta^{(2)}_{\text{ideal}} f(x)\Big|_{x=0} = c_0 f(0),$$

where

$$c_0 \equiv \frac{2}{a^2}\left\{\ldots - \frac{1}{16} + \frac{1}{9} - \frac{1}{4} + 1 - \frac{\pi^2}{6} + 1 - \frac{1}{4} + \frac{1}{9} - \frac{1}{16} + \ldots\right\}. \tag{4}$$

But this is simply an infinite sum of numerical factors, which needs to be only done once. Specifically, (4) is equivalent to

$$c_0 = \frac{2}{a^2}\left\{2\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n^2} - \frac{\pi^2}{6}\right\}.$$

Fortunately, the mathematicians have worked out this infinite sum for us, namely,

$$\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n^2} \equiv \eta(2) = \frac{\pi^2}{12}. \tag{5}$$

Thus, we find

$$c_0 \equiv 0,$$

and hence the ideal SLAC second-derivative of any function defined on a lattice with just one site, with periodic boundary conditions applied to both the function *and the operator*, is identically zero, as argued above.

3. A more realistic example

Let us now consider a more realistic example. For simplicity, let's consider a one-dimensional lattice with, say, $N = 100$ sites. Let us also go back to considering the *first*-derivative of some function $f(x)$ defined on the lattice. Now, since we are assuming periodic boundary conditions, it doesn't really matter how we label the 100 lattice sites relative to the site that we wish to compute the derivative at; but, for definiteness, let us label them from $n = -49$ through $n = +50$ inclusive, with $n = 0$ being the site that we wish to compute the first-derivative at. Now, the SLAC derivative operator (1) tells us to compute differences for increasing distances from $n = 0$, weighting the difference at distance n by $(-1)^{n+1}/na$. In [1], we simply assumed that we should stop when we get to the difference at $n = \pm 49$, since there is no $n = -50$. Let us consider, as an arbitrary example, the lattice position at $n = +43$. The contribution to the sum (1) from this position, according to the truncated prescription of [1], is simply

$$\frac{1}{43a} f(x_{43}).$$

We now wish to apply periodic boundary conditions to this derivative operation. Let us continue to concentrate on the position at $n = +43$. When the derivative operation "runs" through the lattice sites a second time, we will return to this same position, $n = +43$, after going a further distance of $N = 100$ lattice sites. This implies a contribution to the sum in (1) of the amount

$$\frac{1}{143a} f(x_{143} \equiv x_{43}).$$

After another "run" through the lattice sites, we will add a further contribution of

$$\frac{1}{243a} f(x_{43}).$$

Thus, continuing on this process *ad infinitum*, the overall contribution to the sum in (1) will simply be

$$\frac{1}{a}\left\{\frac{1}{43} + \frac{1}{143} + \frac{1}{243} + \frac{1}{343} + \ldots\right\} f(x_{43}).$$

It might seem that the coefficient of this term is simply the coefficient c_{43} that we seek to evaluate. However, we have a problem: this infinite sum is *divergent*, as can be seen from the fact that $1/43 > 1/100$, $1/143 > 1/200$, $1/243 > 1/300$, and so on, so that

$$\begin{aligned}\frac{1}{43} + \frac{1}{143} + \frac{1}{243} + \frac{1}{343} + \ldots &> \frac{1}{100} + \frac{1}{200} + \frac{1}{300} + \frac{1}{400} + \ldots \\ &= \frac{1}{100}\left\{1 + \frac{1}{2} + \frac{1}{3} + \frac{1}{4} + \ldots\right\},\end{aligned}$$

and this last sum is logarithmically divergent.

What has gone wrong? Obviously, the correct coefficient cannot be infinite. The problem is that we have only considered one half of the derivative operation expressed in (1), namely, that for positive n. We have forgotten that, in travelling backwards along the lattice for *negative* n, and applying periodic boundary conditions at the boundary which we are taking to occur after $n = -49$, we will also "run past" the position at $n = +43$. Specifically, the position $n = -57$ is, by the periodic boundary conditions, identically equivalent to $n = +43$, and this term in (1) will contribute an amount

$$-\frac{1}{57a} f(x_{-57} \equiv x_{43}).$$

Going back another $N = 100$ lattice sites, we will also find a contribution of

$$-\frac{1}{157a} f(x_{-157} \equiv x_{43}),$$

and so on. Thus, we find that the true expression for c_{43} is simply

$$c_{43} = \frac{1}{a}\left\{\frac{1}{43} - \frac{1}{57} + \frac{1}{143} - \frac{1}{157} + \frac{1}{243} - \frac{1}{257} + \ldots\right\}. \tag{6}$$

It is straightforward to see that this alternating series is now convergent; for example, by noting that $1/43 < 1/25$, $1/57 < 1/50$, $1/143 < 1/75$, and so on, so that

$$c_{43} < \frac{1}{a}\left\{\frac{1}{25} - \frac{1}{50} + \frac{1}{75} - \frac{1}{100} + \ldots\right\} = \frac{1}{25a}\left\{1 - \frac{1}{2} + \frac{1}{3} - \frac{1}{4} + \ldots\right\} = \frac{\ln 2}{25a} < \infty.$$

Now, you may have noted that, in "wrapping around" the $N = 100$ lattice sites in the above, the fact that N was *even* meant that the sign of the contribution to (1) in any "run" through the lattice (in one direction) was the same as any other "run" through the lattice (in that same direction). How would the situation change if N were *odd*? To examine this situation, let us consider the example of $N = 101$, and let us continue to concentrate our attention on the position $n = +43$. Going through the positive-n terms in (1), we will pick up contributions of

$$\frac{1}{a}\left\{\frac{1}{43} - \frac{1}{144} + \frac{1}{245} - \frac{1}{346} + \ldots\right\}, \tag{7a}$$

where the minus signs arise because the terms in (1) for *even* positive n come in with the minus signs. This sum is now, by itself, convergent. However, to obtain c_{43} we still need to add in the contributions from the negative-n terms in (1). The periodic boundary conditions now tell us that the position $n = -58$ is equivalent to $n = 43$ (because $43 + 58 = 101$), and the coefficient of $f(x - 58a)$ in (1) is positive, so we will obtain the contribution

$$\frac{1}{a}\left\{\frac{1}{58} - \frac{1}{159} + \frac{1}{260} - \frac{1}{261} + \ldots\right\}, \tag{7b}$$

which is also, by itself, convergent.

4. An example of the second derivative

The same process as outlined in the example above can be applied to the second-derivative operator (2) (and, indeed, any higher-order derivative that may be desired). Let us go back to the example of $N = 100$, and consider again the position $n = +43$. Under periodic boundary conditions, the terms in (2) for positive n that contribution to this position are just

$$\frac{2}{a^2}\left\{\frac{1}{43^2} + \frac{1}{143^2} + \frac{1}{243^2} + \frac{1}{343^2} + \ldots\right\} f(x_{43}). \tag{8a}$$

Because these denominators are squared, rather than linear, this sum converges on its own. The negative-n terms in (2) that contribute to this position are just

$$\frac{2}{a^2}\left\{\frac{1}{57^2}+\frac{1}{157^2}+\frac{1}{257^2}+\frac{1}{357^2}+\ldots\right\}f(x_{43}), \tag{8b}$$

which also converges. For even N, these two sums contribute with the same sign.

It is clear that the same of calculation would also apply for the case of $n=+50$, which is "half a lattice away" from $n=0$, even though there is no corresponding $n=-50$ (which is, by the periodic boundary conditions, equivalent to $n=+50$); for this position, the two sums of the form (8a) and (8b) will be identical.

Now, because the central ($n=0$) term in the operator (2) is nonzero, and because each term for $-n$ comes in with the *same* sign as that for $+n$, we also need to separately compute the coefficient c_0 under the assumption of periodic boundary conditions. For the case of $N=100$, we simply obtain

$$c_0=\frac{2}{a^2}\left\{-\frac{\pi^2}{6}-\frac{2}{100^2}-\frac{2}{200^2}-\frac{2}{300^2}-\ldots\right\}, \tag{9}$$

where the factor of 2 in each term arises from the fact that we are adding in the contributions from both positive-n and negative-n (which are both one lattice "revolution" away).

Let us now go back to the odd-N example of $N=101$. For the position $n=+43$, the positive-n terms that contribute are just

$$\frac{2}{a^2}\left\{\frac{1}{43^2}-\frac{1}{144^2}+\frac{1}{245^2}-\frac{1}{346^2}+\ldots\right\}f(x_{43}), \tag{10a}$$

and the negative-n terms that contribute are just

$$\frac{2}{a^2}\left\{-\frac{1}{58^2}+\frac{1}{159^2}-\frac{1}{260^2}+\frac{1}{361^2}+\ldots\right\}f(x_{43}). \tag{10b}$$

The extra minus signs that arise from using an odd number of lattice sites make the overall sum converge more quickly than for an even value of N. For the "central" coefficient c_0, we now obtain

$$c_0=\frac{2}{a^2}\left\{-\frac{\pi^2}{6}+\frac{2}{101^2}-\frac{2}{202^2}+\frac{2}{303^2}-\ldots\right\}, \tag{11}$$

where the minus signs are again due to the fact that we are alternately picking up the odd and even terms in (2).

5. Exact, general expressions for the finite-lattice SLAC derivative operators

Let us now make use of the examples provided in Secs. 3 and 4 to guide us in constructing, from first principles, the general expressions for the SLAC derivative operators on a finite lattice on which we assume periodic boundary conditions.

Let us start with the first-derivative operator. We can write the expression (6) for c_{43} with $N=100$ in the form

$$^{(1)}c_{43}^{100}=\frac{1}{a}\sum_{k=0}^{\infty}\left\{\frac{1}{100k+43}-\frac{1}{100k+57}\right\},$$

where I am using the notation

$$ {}^{(m)}C_n^N $$

for the coefficient of the ideal SLAC m-th derivative operator at position n for a finite lattice of N lattice sites. If we had chosen a general lattice position n (positive) rather than the particular choice of $n = 43$, we would have obtained

$$ {}^{(1)}C_{n\ \text{positive}}^{100} = \frac{(-1)^{n+1}}{a} \sum_{k=0}^{\infty} \left\{ \frac{1}{100k+n} - \frac{1}{100k+100-n} \right\}, $$

where the alternating sign out the front is due to the alternating sign in (1). Clearly, if we were to have a general (even) number N of lattice sites, this result would become

$$ {}^{(1)}C_{n\ \text{positive}}^{N\ \text{even}} = \frac{(-1)^{n+1}}{a} \sum_{k=0}^{\infty} \left\{ \frac{1}{Nk+n} - \frac{1}{Nk+N-n} \right\}. $$

If we factorise out a factor of N from each of these denominators, we obtain

$$ {}^{(1)}C_{n\ \text{positive}}^{N\ \text{even}} = \frac{(-1)^{n+1}}{Na} \sum_{k=0}^{\infty} \left\{ \frac{1}{k+n/N} - \frac{1}{k+1-n/N} \right\}. $$

Fortunately, the mathematicians have again evaluated this infinite sum for us, and it yields a remarkably simple result:

$$ \sum_{k=0}^{\infty} \left\{ \frac{1}{k+n/N} - \frac{1}{k+1-n/N} \right\} = \pi \cot\left(\frac{\pi n}{N} \right). \qquad (12) $$

Thus, we find that

$$ {}^{(1)}C_{n\ \text{positive}}^{N\ \text{even}} = (-1)^{n+1} \frac{\pi}{Na} \cot\left(\frac{\pi n}{N} \right). $$

Let us now consider a negative value of n (but keeping N even). From (1), all of the terms come in with the opposite sign, but since $(-1)^{-n+1} \equiv (-1)^{n+1}$ and $\cot(-x) \equiv -\cot x$, we can see that the same expression can be used for negative n. Hence, in general (for even N), we have

$$ {}^{(1)}C_{n\neq 0}^{N\ \text{even}} = (-1)^{n+1} \frac{\pi}{Na} \cot\left(\frac{\pi n}{N} \right). \qquad (13) $$

It is clear that, for small n (namely, far from the application of the periodic boundary conditions), this formula approaches the infinite lattice result (1), because $\cot x \equiv 1/\tan x \sim 1/x$ for small x, and hence

$$ {}^{(1)}C_{n\neq 0}^{N\ \text{even}} \to \frac{(-1)^{n+1}}{na} \quad \text{as} \quad \frac{n}{N} \to 0. $$

On the other hand, near the edge of the application of periodic boundary conditions, namely, $n \to N/2$, the absolute values of the coefficients (13) approach zero linearly with $(N/2 - n)$.

Let us now consider the case of an odd number of lattice sites N. We again start at a position of positive n. The example (7a) shows us that the positive-n terms in (1) themselves contribute an amount that can be written

$$\frac{1}{a}\lim_{M\to\infty}\left\{2\sum_{k=0}^{M}\frac{1}{202k+43}-\sum_{k=0}^{2M}\frac{1}{101k+43}\right\},$$

where we have written the two sums in this way (the first sum contributing to every *other* term in (7a), with the second sum contributing to *every* term) to maintain the closest possible relationship with the even-N analysis above. (The limiting process is necessary because each sum does not individually converge.) Likewise, by (7b) we see that the negative-n terms in (1) contribute an amount

$$\frac{1}{a}\lim_{M\to\infty}\left\{2\sum_{k=0}^{M}\frac{1}{202k+58}-\sum_{k=0}^{2M}\frac{1}{101k+58}\right\}.$$

Putting these together, we then have

$${}^{(1)}c_{43}^{101}=\frac{1}{a}\lim_{M\to\infty}\left\{\sum_{k=0}^{M}\left(\frac{2}{202k+43}+\frac{2}{202k+58}\right)-\sum_{k=0}^{2M}\left(\frac{1}{101k+43}+\frac{1}{101k+58}\right)\right\}.$$

Generalising to the case of general (odd) N, and positive n, we clearly obtain

$${}^{(1)}c_{n\text{ positive}}^{N\text{ odd}}=\frac{(-1)^{n+1}}{a}\lim_{M\to\infty}\left\{\sum_{k=0}^{M}\left(\frac{2}{2Nk+n}+\frac{2}{2Nk+N-n}\right)-\sum_{k=0}^{2M}\left(\frac{1}{Nk+n}+\frac{1}{Nk+N-n}\right)\right\}.$$

Again factorising N from these denominators, we then obtain

$${}^{(1)}c_{n\text{ positive}}^{N\text{ odd}}=\frac{(-1)^{n+1}}{Na}\lim_{M\to\infty}\left\{\sum_{k=0}^{M}\left(\frac{1}{k+n/2N}+\frac{1}{k+1/2-n/2N}\right)-\sum_{k=0}^{2M}\left(\frac{1}{k+n/N}+\frac{1}{k+1-n/N}\right)\right\}.$$

Fortunately, the mathematicians have also evaluated this combination of infinite limits of sums for us, and again it is a remarkably simple result:

$$\lim_{M\to\infty}\left\{\sum_{k=0}^{M}\left(\frac{1}{k+n/2N}+\frac{1}{k+1/2-n/2N}\right)-\sum_{k=0}^{2M}\left(\frac{1}{k+n/N}+\frac{1}{k+1-n/N}\right)\right\}=\pi\csc\left(\frac{\pi n}{N}\right). \tag{14}$$

We thus find that

$${}^{(1)}c_{n\text{ positive}}^{N\text{ odd}}=(-1)^{n+1}\frac{\pi}{Na}\csc\left(\frac{\pi n}{N}\right).$$

As before, this expression is odd under $n \to -n$, in accordance with (1), and so for a general position n (for odd N) we have the result

$$ {}^{(1)}c_{n\neq 0}^{N\,\mathrm{odd}} = (-1)^{n+1}\frac{\pi}{Na}\csc\left(\frac{\pi n}{N}\right). \tag{15} $$

Again, since $\csc x \equiv 1/\sin x \sim 1/x$ for small x, we find that far from the application of periodic boundary conditions we regain the infinite-lattice result:

$$ {}^{(1)}c_{n\neq 0}^{N\,\mathrm{odd}} \to \frac{(-1)^{n+1}}{na} \quad \text{as} \quad \frac{n}{N} \to 0. $$

However, in contrast to the case of even N, for odd N we find that, near the edge of the application of periodic boundary conditions, namely, $n \to N/2$, the absolute value of ${}^{(1)}c_{n\neq 0}^{N\,\mathrm{odd}}$ approaches the finite value π/Na. If it weren't for the periodic boundary conditions, the absolute value of the coefficient function at the limit of this boundary (between lattice sites) would only have been $1/na = 2/Na$; thus, the applications of periodic boundary conditions for odd N has actually *increased* the magnitude of the coefficient function at the boundary by a factor of $\pi/2$, or around a 57% increase. Indeed, this is a general phenomenon:

$$ \left|{}^{(1)}c_{n\neq 0}^{N\,\mathrm{odd}}\right| > \frac{1}{na}, $$

whereas

$$ \left|{}^{(1)}c_{n\neq 0}^{N\,\mathrm{even}}\right| < \frac{1}{na}, $$

although in each case the magnitude of the inequality is relatively mild, as we shall see shortly in Sec. 6.

Let us now turn to the second-derivative operator. The expressions (8a) and (8b) clearly combine to give us

$$ {}^{(2)}c_{43}^{100} = \frac{2}{a^2}\sum_{k=0}^{\infty}\left\{\frac{1}{(100k+43)^2} + \frac{1}{(100k+57)^2}\right\}. $$

Going to general (even) N and general $n \neq 0$ (positive or negative, since they come in with the same sign for the second-derivative), we clearly have

$$ {}^{(2)}c_{n\neq 0}^{N\,\mathrm{even}} = \frac{2(-1)^{n+1}}{a^2}\sum_{k=0}^{\infty}\left\{\frac{1}{(Nk+n)^2} + \frac{1}{(Nk+N-n)^2}\right\}, $$

and factorising out N^2 from the denominators we have

$$ {}^{(2)}c_{n\neq 0}^{N\,\mathrm{even}} = \frac{2(-1)^{n+1}}{(Na)^2}\sum_{k=0}^{\infty}\left\{\frac{1}{(k+n/N)^2} + \frac{1}{(k+1-n/N)^2}\right\}. $$

Again, the mathematicians give us a magic result for the infinite sum:

$$ \sum_{k=0}^{\infty}\left\{\frac{1}{(k+n/N)^2} + \frac{1}{(k+1-n/N)^2}\right\} = \pi^2\csc^2\left(\frac{\pi n}{N}\right), \tag{16} $$

so that

$$ {}^{(2)}c_{n\neq 0}^{N\,\text{even}} = 2(-1)^{n+1}\left(\frac{\pi}{Na}\right)^2 \csc^2\left(\frac{\pi n}{N}\right). \tag{17} $$

From the way we have constructed it, this expression clearly also applies to the (single) position $n = +N/2$, that is half a lattice away from the position $n = 0$ at which we are applying the derivative. Clearly, far from the application of periodic boundary conditions, we again regain from (17) the infinite-lattice result (2).

For $n = 0$, the expression (9) can be written

$$ {}^{(2)}c_{0}^{N\,\text{even}} = -\frac{2}{a^2}\left\{\frac{\pi^2}{6} + \frac{2}{N^2}\sum_{k=1}^{\infty}\frac{1}{k^2}\right\}, $$

and since

$$ \sum_{k=1}^{\infty}\frac{1}{k^2} \equiv \zeta(2) = \frac{\pi^2}{6}, $$

we find

$$ {}^{(2)}c_{0}^{N\,\text{even}} = -\frac{\pi^2}{3a^2}\left(1 + \frac{2}{N^2}\right). \tag{18} $$

It can be shown that the additional contribution here for finite N is equal to the difference between the finite-lattice result (17) and the infinite-lattice result (2) for $n \neq 0$ if we assume the expression to hold true for real n and take the limit $n \to 0$.

Finally, we consider the case of odd N. The sum in (10a) can be written

$$ \frac{2}{a^2}\left\{2\sum_{k=0}^{\infty}\frac{1}{(202k+43)^2} - \sum_{k=0}^{\infty}\frac{1}{(101k+43)^2}\right\}, $$

where in this case we don't need to be careful about the limiting process because each sum is separately convergent. Likewise, the sum in (10b) can be written

$$ -\frac{2}{a^2}\left\{2\sum_{k=0}^{\infty}\frac{1}{(202k+58)^2} - \sum_{k=0}^{\infty}\frac{1}{(101k+58)^2}\right\}, $$

Combining these expressions, we then have

$$ {}^{(2)}c_{43}^{101} = \frac{2}{a^2}\sum_{k=0}^{\infty}\left\{\frac{2}{(202k+43)^2} - \frac{2}{(202k+58)^2} - \frac{1}{(101k+43)^2} + \frac{1}{(101k+58)^2}\right\}. $$

For general (odd) N and $n \neq 0$, this becomes

$$ {}^{(2)}c_{n\neq 0}^{N\,\text{odd}} = \frac{2(-1)^{n+1}}{a^2}\sum_{k=0}^{\infty}\left\{\frac{2}{(2Nk+n)^2} - \frac{2}{(2Nk+N-n)^2} - \frac{1}{(Nk+n)^2} + \frac{1}{(Nk+N-n)^2}\right\}, $$

and on factorising out N^2 we get

$$
{}^{(2)}c_{n\neq 0}^{N\,\mathrm{odd}} = \frac{2(-1)^{n+1}}{(Na)^2}\sum_{k=0}^{\infty}\biggl\{\frac{1/2}{(k+n/2N)^2} - \frac{1/2}{(k+1/2-n/2N)^2} - \frac{1}{(k+n/N)^2} + \frac{1}{(k+1-n/N)^2}\biggr\}.
$$

Again, the mathematicians have evaluated this sum for us:

$$
\sum_{k=0}^{\infty}\biggl\{\frac{1/2}{(k+n/2N)^2} - \frac{1/2}{(k+1/2-n/2N)^2} - \frac{1}{(k+n/N)^2} + \frac{1}{(k+1-n/N)^2}\biggr\} = \pi^2 \csc\Bigl(\frac{\pi n}{N}\Bigr)\cot\Bigl(\frac{\pi n}{N}\Bigr), \tag{19}
$$

so that

$$
{}^{(2)}c_{n\neq 0}^{N\,\mathrm{odd}} = 2(-1)^{n+1}\Bigl(\frac{\pi}{Na}\Bigr)^2 \csc\Bigl(\frac{\pi n}{N}\Bigr)\cot\Bigl(\frac{\pi n}{N}\Bigr). \tag{20}
$$

For $n = 0$, the expression (11) can be written

$$
{}^{(2)}c_{0}^{N\,\mathrm{odd}} = -\frac{2}{a^2}\biggl\{\frac{\pi^2}{6} - \frac{2}{N^2}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^2}\biggr\},
$$

and so, using (5), we find

$$
{}^{(2)}c_{0}^{N\,\mathrm{odd}} = -\frac{\pi^2}{3a^2}\Bigl(1 - \frac{1}{N^2}\Bigr). \tag{21}
$$

The expressions (20) and (21) are in agreement with those listed explicitly by Drell, Weinstein and Yankielowicz [2] in the first of their seminal papers. Note, however, that these authors only considered the case of an odd number of lattice sites (which is written as $2N + 1$ in their notation); and as no explicit expressions for the first-derivative operation in position space are provided in [2], further comparisons with the expressions listed above are not possible.

Clearly, the expressions above for the second-derivative operator on finite lattices also reduce to the infinite-lattice results for $n/N \to 0$, as was the case for the first-derivative operators. Near the application of periodic boundary conditions, the even-N expression (17) approaches a finite limit, whereas the odd-N expression (20) approaches zero, which is a reversal of rôles from the case of the first-derivative operators (for which the even-N coefficient vanished linearly, and the odd-N coefficient approached a finite value).

6. Stochastic implementation of the finite-lattice SLAC derivative operators

Let us now turn to the reason why we are considering the practical implementation of the SLAC derivative operators at all, namely, my proposal in [1] that they be implemented in a stochastic fashion. How must this proposal be modified to accommodate the corrections obtained in Sec. 5 to incorporate exactly the implementation of periodic boundary conditions for a finite lattice?

I propose the following: that the probabilistic weight assigned to the computation of any difference (sum) in the first (second) SLAC derivative operator at distance n be calculated using the *same* value $1/n$ $(2/n^2)$ as was proposed in [1] on the basis of the truncation of the infinite-lattice operators, but that the result of such sum (difference)—if calculated—be multiplied by a "correction factor" that incorporates exactly the effects of restricting the formalism to a finite lattice and applying periodic boundary conditions.

My reasons for proposing this solution are twofold. Firstly, as noted in Sec. 5 (and as will become explicit below), the required "correction factors" are, in all cases, simply numbers of order unity, which do not affect the fluctuation properties of the proposed stochastic implementation in any functionally critical fashion; we simply weight some positions a little more, or less, than for the case of an infinite lattice. Secondly, it is clear that if this is all that we need to do, then it would be silly to tamper with the extraordinarily efficient method of random selection described in [1] for probabilistic weight functions of $1/n$ or $2/n^2$, because the decision to compute or not compute needs to be made for every distance n for every application of the derivative operator, and may, if blown out to a set of floating-point computations, become the time-critical part of the algorithm that would limit its practical implementation on a digital computer. (It is important to note that the floating-point multiplication of the result of the sum or difference by the correction factor need only be done *if the sum or difference is actually computed*, and hence the average number of extra floating-point operations according to this proposed solution is itself proportional to $\ln N$, rather than being proportional to N if the probabilistic weights were instead modified.)

From the results obtained in Sec. 5, it is simple to write down expressions for these correction factors. If we define

$$^{(m)}\kappa_n^N$$

to be the correction factor for the distance-n sum or difference for the m-th order SLAC derivative operator on a (one-dimensional) lattice of N sites, then clearly

$$^{(m)}\kappa_n^N \equiv \frac{^{(m)}c_n^N}{^{(m)}c_n^\infty}.$$

From the results (13), (15), (17) and (20) we then simply have

$$^{(1)}\kappa_{n>0}^{N\,\mathrm{even}} = \alpha \cot \alpha, \tag{22a}$$
$$^{(1)}\kappa_{n>0}^{N\,\mathrm{odd}} = \alpha \csc \alpha, \tag{22b}$$
$$^{(2)}\kappa_{n>0}^{N\,\mathrm{even}} = \alpha^2 \csc^2 \alpha, \tag{22c}$$
$$^{(2)}\kappa_{n>0}^{N\,\mathrm{odd}} = \alpha^2 \csc \alpha \cot \alpha, \tag{22d}$$

where

$$\alpha \equiv \frac{\pi n}{N} \qquad \left(0 < \alpha \le \frac{\pi}{2}\right), \tag{23}$$

and from (18) and (21) we have

$$^{(2)}\kappa_0^{N\,\mathrm{even}} = 1 + \frac{2}{N^2}, \tag{24a}$$
$$^{(2)}\kappa_0^{N\,\mathrm{odd}} = 1 - \frac{1}{N^2}. \tag{24b}$$

As noted above, the expressions (22) are relatively "boring" functions of α. They all approach unity for $\alpha \to 0$. For $\alpha \to \pi/2$, the expressions (22a) and (22d), involving $\cot\alpha$, fall smoothly to zero, whereas the expressions (22b) and (22c) rise to the finite values $\pi/2$ and $\pi^2/4$ respectively.

7. Conclusions

We have found that it is relatively easy to get a good physical understanding of the SLAC derivative operators on *finite* one-dimensional lattices, in position space, by considering explicitly the imposition of periodic boundary conditions on the corresponding expressions for infinite lattices. In all cases this leads to small adjustments of coefficients, which can be written down in a very simple form. There are qualitative differences between these correction factors depending on whether the lattice has an odd or an even number of sites, but in all cases the factors are numbers of order unity. This means that the stochastic implementation of the operators proposed in [1] requires only superficial changes in order to make the operators completely optimal for any finite lattice.

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References

[1] J. P. Costella, `hep-lat/0207008`.
[2] S. D. Drell, M. Weinstein and S. Yankielowicz, *Phys. Rev. D* **14** (1976) 487; 1627.