Fourier acceleration in lattice gauge theories. I. Landau gauge fixing

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Fourier acceleration is a useful technique which can be applied to many different numerical algorithms in order to alleviate the problem of critical slowing down. Here we describe its application to an optimization problem in the simulation of lattice gauge theories, that of gauge fixing a configuration of link fields to the Landau gauge ($\partial_\mu A^\mu = 0$). We find that a steepest-descents method of gauge fixing link fields at $\beta = 5.8$ on an 8^4 lattice can be made 5 times faster using Fourier acceleration. This factor will grow as the volume of the lattice is increased. We also discuss other gauges that are useful to lattice-gauge-theory simulations, among them one that is a combination of the axial and Landau gauges. This seems to be the optimal gauge to impose for the Fourier acceleration of two other important algorithms, the inversion of the fermion matrix and the updating of gauge field configurations.

I. INTRODUCTION

Many types of numerical computation that involve iterative algorithms suffer a severe problem from the phenomenon of critical slowing down. It typically takes the form that the number of iterations required to solve the problem grows as some positive power of the number of sites used in discretizing the system, the volume V. Since the computer time required for one iteration also (unavoidably) grows at least as fast as V, computations on large systems, presumably the most relevant physically, become prohibitively time consuming.

Iterative algorithms become very slow when the change of the system under one iteration of the algorithm is governed by a matrix which has a large range of eigenvalues. Critical slowing down occurs when this range increases with V. The eigenvectors corresponding to the small eigenvalues lag behind the others as the computation progresses and control the speed of convergence. The solution is to adjust the matrix ("precondition it") so that all of its eigenvalues become approximately equal to the largest one, but in such a way that the final answer is not affected. The evolution of the system with computer time is radically affected, however, and should be speeded up by the ratio of the largest to the smallest eigenvalues of the relevant matrix. Any volume dependence in the number of iterations required will also be removed.

This acceleration scheme will work well if the computational cost of preconditioning the matrix is small—if it grows only as a single power of the volume, for example. In physical systems it is often true that the matrix which governs the evolution is, at least approximately, diagonal in momentum space. Critical slowing down is a consequence of new eigenvalues at low momentum (in lattice units) appearing as the volume is increased. Preconditioning by Fourier acceleration then involves multiplication by a diagonal matrix in momentum space[1,2] and has a cost which grows as $V \ln(V)$, being the cost of a fast Fourier transform (FFT).

In this and the following two papers[3,4] we discuss the application of Fourier acceleration to numerical algorithms for optimization, matrix inversion, and generating lattice field configurations. We have found a consid-

erable gain in the computational speed for the numerical simulation of lattice gauge theories[5] and we believe that there are similar gains to be made in many other areas (see, for example, Ref. 6).

This paper describes the use of Fourier acceleration in an optimization algorithm, specifically that used for fixing lattice gauge field configurations to the Landau gauge. Section II introduces the method of Fourier acceleration applied to a simple optimization problem and then in Sec. III we discuss the algorithm for transforming a lattice gauge field configuration to Landau gauge. Finally we discuss the uses of gauge fixing in simulations of lattice gauge theories. In particular we describe a gauge in which it is possible to Fourier accelerate both the algorithm which calculates fermion propagators and that which generates an ensemble of gauge field configurations. This gauge is a combination of axial and Landau gauges and we have called it the "AL gauge."

II. OPTIMIZATION AND FOURIER ACCELERATION

As a simple example of an optimization problem, consider the transformation of an electromagnetic vector potential $A_\mu(x)$ to the Landau gauge, $\partial_\mu A^\mu=0$. This can be considered as a minimization of

$$F=\int d^4x\ A^g_\mu(x)A^{g\mu}(x) \tag{2.1}$$

in the space of gauge-equivalent fields $A^g_\mu(x)$. $A_\mu(x)$ transforms under a gauge transformation g as

$$A_\mu(x)\rightarrow A^g_\mu(x)=A_\mu(x)-\partial_\mu\chi(x)\ . \tag{2.2}$$

At each step of the gauge-fixing algorithm we want to select the field $\chi(x)$ so that

$$\int d^4x\ A_\mu(x)A^\mu(x) \geq \int d^4x\,[A_\mu(x)-\partial_\mu\chi(x)][A^\mu(x)-\partial^\mu\chi(x)]\ . \tag{2.3}$$

This is achieved for small enough values of α by setting

$$\chi(x)=-\alpha\partial_\mu A^\mu(x)\ , \tag{2.4}$$

since the integrand on the right-hand side of Eq. (2.3) becomes

$$A_\mu A^\mu-2\alpha(\partial_\mu A^\mu)^2+\alpha^2(\partial_\mu\partial^\nu A_\nu\partial^\mu\partial_\gamma A^\gamma)\ . \tag{2.5}$$

The gauge-fixing procedure is then carried out as follows: at each step $\chi(x)$ is calculated from Eq. (2.4) and then the gauge transformation of Eq. (2.2) is applied to the fields $A_\mu(x)$. As this step is repeated the function F of Eq. (2.1) will converge monotonically to a minimum value if α is small enough. The value of $\partial_\mu A^\mu$ will be zero at this minimum. This algorithm is a steepest-descents or Jacobi method of optimization since at each stage a step is taken along the direction of the local gradient $\partial F/\partial\chi(x)$, calculated at $\chi=0$.

It is clear that this algorithm shows critical slowing down if we examine the behavior under the iteration scheme of $\partial_\mu A^\mu(x)$. At the nth iteration

$$\partial_\mu A^{\mu(n)}(x)=\partial_\mu A^{\mu(n-1)}(x)+\alpha\partial^2\partial_\mu A^{\mu(n-1)}(x)\ . \tag{2.6}$$

Solving in momentum space and denoting the Fourier transform by a tilde,

$$\partial\cdot\tilde{A}^{(n)}(p)=[\partial\cdot\tilde{A}^{(0)}(p)](1-\alpha p^2)^n \approx[\partial\cdot\tilde{A}^{(0)}(p)]\exp(-\alpha p^2 n)\ \text{ for large } n\ . \tag{2.7}$$

The decay rates of the different momentum components of $\partial_\mu A^\mu$ are controlled by the eigenvalues of the operator $-\partial^2$. These eigenvalues will be called p^2. Since we need $\alpha<1/p^2_{\max}$ for stability, the eigenvector corresponding to the lowest nonzero value of p^2, $p^2_{\min}$, will have a decay time

$$\tau_{\min}\propto\frac{p^2_{\max}}{p^2_{\min}}\ . \tag{2.8}$$

If we discretize spacetime into a hypercubic lattice of points with L points on a side then $p^2_{\min}\propto 1/L^2$. The computation time to reach $\partial_\mu A^\mu=0$ will then grow as VL^2 or, in four dimensions, as $V^{3/2}$.

Fourier acceleration enables the step taken at each iteration by the eigenvectors which lag behind to be made larger. The step size α becomes a diagonal matrix in momentum space, $\alpha(p)$ with

$$\alpha(p)=\alpha\frac{p^2_{\max}}{p^2}\ . \tag{2.9}$$

The nth iteration of the scheme with Fourier acceleration is

$$A^{\mu(n)}(x)=A^{\mu(n-1)}(x)+\hat{F}^{-1}\alpha\frac{p^2_{\max}}{p^2}\hat{F}\partial^\mu\partial_\nu A^{\nu(n-1)}(x)\ , \tag{2.10}$$

where $\hat{F}$ represents an FFT. Now all momentum components of $\partial_\mu A^\mu$ converge to zero at the same rate since the matrix controlling the convergence is proportional to the unit matrix. In fact we can fix to Landau gauge in one step in this (admittedly trivial) case.

The cost of an iteration of this algorithm will have a part proportional to $V\ln(V)$ from the FFT and an additional part proportional to V from the rest of the calculation. Either of these parts may dominate at a given value of V depending on program efficiency. The number of iterations is now independent of V, however, so either dependence is to be preferred to the $V^{3/2}$ growth in the cost of the unaccelerated algorithm.

III. LANDAU GAUGE FIXING ON THE LATTICE

A lattice gauge theory is formulated in terms of matrices U which are elements of the gauge group and which sit on the links of the lattice. Our work has been concerned mainly with gauge groups SU(N_C) and particularly SU(3), relevant to QCD. The results we present will be for this group with link matrices in the fundamental representation.

To fix a lattice version of the Landau gauge we max-

imize the function F_L which, by analogy with Eq. (2.1), is given by

$$F_L=\frac{1}{2N_C}\frac{1}{4V}\sum_{\mu,x}\mathrm{Tr}[U_\mu^g(x)+U_\mu^{g\dagger}(x)] \tag{3.1}$$

in the space of gauge-equivalent fields $U_\mu^g(x)$. $U_\mu(x)$ transforms under a gauge transformation as

$$U_\mu^g(x)=G(x)U_\mu(x)G^\dagger(x+\mu)\ , \tag{3.2}$$

where the matrices $G(x)$ belong to the same representation of the gauge group as $U_\mu(x)$ and sit on the sites of the lattice.

The naive steepest-descents method chooses $G(x)$ at each step of the iterative procedure to be

$$G(x)=\exp\left\{\frac{\alpha}{2}\left[\sum_\nu\left[\Delta_{-\nu}(U_\nu(x)-U_\nu^\dagger(x))-\frac{1}{N_C}\mathrm{Tr}[\Delta_{-\nu}(U_\nu(x)-U_\nu^\dagger(x))]\right]\right]\right\}, \tag{3.3}$$

where

$$\Delta_{-\nu}(U_\mu(x))=U_\mu(x-\hat{\nu})-U_\mu(x)\ . \tag{3.4}$$

This follows from differentiating F_L with respect to $w_j(x)$ where $G(x)=\exp(iw_jT^j)$. An expansion of the exponential in Eq. (3.3) to leading order in a followed by reunitarization of $G(x)$ is sufficient for numerical purposes.

The function F_L will increase monotonically as the algorithm proceeds and at its maximum $G(x)$ will be proportional to the unit matrix. Then the matrix

$$\Delta=\sum_\nu[U_\nu(x-\nu)-U_\nu(x)-\mathrm{H.c.}\ -\mathrm{trace}]$$

will be zero. This means that

$$\theta(x)=\mathrm{Tr}[\Delta(x)\Delta^\dagger(x)]=0 \tag{3.5}$$

and

$$\theta=\frac{1}{VN_C}\sum_x\theta(x)=0\ ,$$

the lattice version of $\partial_\mu A^\mu=0$.

This algorithm suffers from critical slowing-down in the same way as the one described in Sec. II. The number of iterations required to fix the gauge grows with the number of sites on the lattice.

The Fourier accelerated algorithm replaces Eq. (3.3) by

$$G(x)=\exp\left[\hat{F}^{-1}\frac{\alpha}{2}\frac{p_{\max}^2a^2}{p^2a^2}\hat{F}\left[\sum_\nu\Delta_{-\nu}(U_\nu(x)-U_\nu^\dagger(x))-\mathrm{trace}\right]\right]\ , \tag{3.6}$$

where p^2 are the eigenvalues of the lattice version of the $(-\partial^2)$ operator and a is the lattice spacing. We use skew-periodic boundary conditions for the gauge field on a hypercubic lattice. If the Fourier transform is defined using $\exp(i2m\pi/L^4)$ then the values of p are given by

$$p^2a^2=4\sum_{\mu=1}^4\sin^2\left[\frac{m\pi}{L^\mu}\right],\quad m=0,\ldots,L^4-1\ , \tag{3.7}$$

where L^μ means L to the power μ. The $p^2=0$ ($m=0$) eigenvalue is adjusted to some nonzero value in Eq. (3.6) to prevent numerical problems. The corresponding eigenvector is irrelevant since it gives no contribution to $G(x)$. This is because on the lattice

$$\sum_x\sum_\nu\Delta_{-\nu}(U_\nu(x))=0 \tag{3.8}$$

corresponding to the continuum integral over a total divergence.

We have tried both the accelerated and unaccelerated algorithms on configurations of link fields obtained from a simulation of SU(3) on an 8^4 lattice with the Wilson action and no fermions. In both cases α should be chosen so as to give the minimum number of iterations without destabilizing the algorithm and causing F_L to fall. We found that a value of α of 0.1 was suitable for the unaccelerated algorithm and 0.08 with acceleration. It is also possible to change the value of α as the algorithm proceeds but we did not find this to be worthwhile. We monitor the value of F_L [Eq. (3.1)] and of θ [Eq. (3.5)].

In Figs. 1 and 2 we show the results of gauge fixing a given configuration, which had been obtained by thermalization at $\beta=5.8$ using an updating algorithm which did not include gauge fixing. The results are typical of the six different configurations that we tested. The value of F_L rose from 0.0 to about 0.83 and the value of θ dropped from around 14 to 0.0 within machine precision. [The value of θ expected for a configuration without gauge fixing is calculated to be $16(1-1/N_C^2)=14.2$ for $N_C=3$.] It is clear from the figures that the Fourier-accelerated algorithm achieves a gauge-fixing to

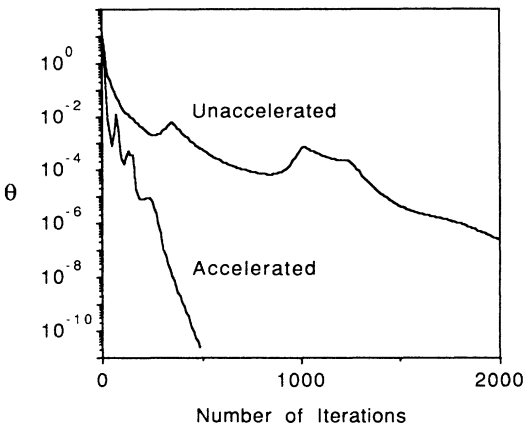

FIG. 1. θ [Eq. (3.5)] plotted as a function of iteration number for gauge fixing an 8^4 configuration of link fields at $\beta=5.8$, with and without Fourier acceleration.

matching precision in about 7 times fewer iterations than the unaccelerated algorithm. Each iteration takes about 1.3 times longer when the FFT's are included but this depends both on the volume of the lattice and the machine being used.

It is evident that large gains are to be made by Fourier acceleration. This will become even more obvious on larger lattices since the number of iterations of the accelerated algorithm is now approximately independent of volume. This has been explicitly checked by going from a 4^4 to an 8^4 lattice when the unaccelerated algorithm required 3–4 times as many iterations. Figure 3 shows a plot of the decay times of the different momentum (p^2a^2) components of $\Theta(m)$, the Fourier transform of $\theta(x)$. Without acceleration, it is clear that the components of $\Theta(m)$ with low values of p^2a^2 converge slowly and hold up the algorithm. As the volume is increased, even smaller values of p^2a^2 will appear and exacerbate the situation. All components of lattice momenta converge at the same rate when acceleration is included.

The Fourier acceleration seems in fact to be more effective than one might expect here. In the Abelian case of Sec. II the critical slowing down was a purely kinematical effect as is clear from Eq. (2.6). Complications arise in a non-Abelian theory because $G(x)$ and $U_\mu(x)$ do not commute. The analog of Eq. (2.2) for a continuum non-Abelian theory is

$$A_\mu^g(x)=A_\mu(x)-D_\mu\chi\ , \tag{3.9}$$

where

$$D_\mu\chi=\partial_\mu\chi-i[A_\mu,\chi]\ , \tag{3.10}$$

and that of Eq. (2.6):

$$\partial_\mu A^{\mu(n)}(x)=\partial_\mu A^{\mu(n-1)}+\alpha(\partial D)\partial_\mu A^{\mu(n-1)}\ . \tag{3.11}$$

It is the eigenvalues of ∂D that are important to critical slowing down, and these depend on the field itself. It appears, however, that the ∂D operator behaves very much like ∂^2 in momentum space but with a modified coefficient. This is seen from Fig. 3 where the decay times of $|\Theta(m)|^2$ to 10% of its original value do not follow $1.15/(\alpha p^2a^2)$ predicted from the continuum Abelian theory [Eq. (2.6)] but instead are 5–10 times longer. When we gauge fix an SU(3) link field configuration with all links close to the unit matrix, so that A_μ is small, then we recover the correlation times of Eq. (2.6). The non-Abelian nature of the fields therefore does play a role in the gauge-fixing algorithm but luckily does not destroy the efficacy of the Fouirer acceleration technique. Indeed Fourier acceleration still works for the gauge fixing of random SU(3) link fields obtained from a hot start.

It is interesting to ask whether the gauge fixing obtained by this algorithm is a complete one, i.e., have all local gauge degrees of freedom been removed? In the continuum there is a Gribov ambiguity[7] associated with Landau gauge which corresponds to zero eigenvalues of the ∂D operator of Eq. (3.11). This means that it is possible to make a local gauge transformation from a configuration satisfying the gauge condition to another one which also satisfies that condition. The Gribov am-

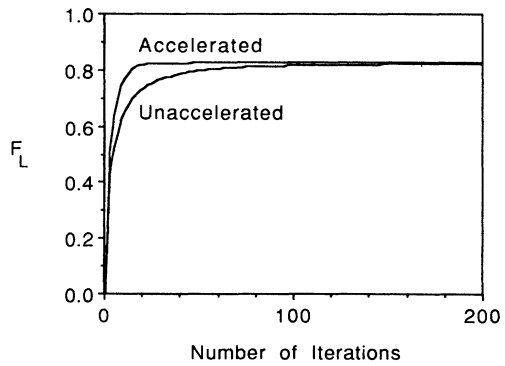

FIG. 2. F_L [Eq. (3.1)] plotted as a function of iteration number for the same configuration as in Fig. 1, with and without Fourier acceleration. Data for only the first 200 of 2000 iterations are shown.

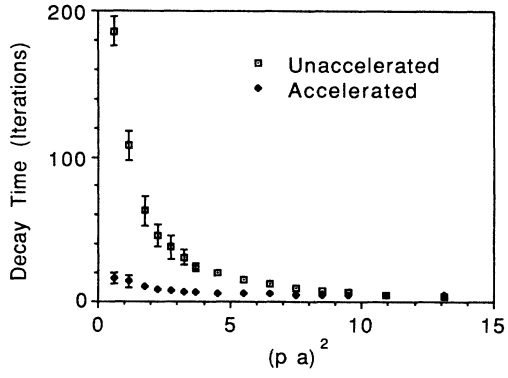

FIG. 3. The time in iterations taken by various momentum components of $|\Theta(m)|^2$ to decay to 10% of their initial value plotted against p^2a^2, the eigenvalue of $(-a^2\partial^2)$ for that value of m.

biguity is intimately related to the problem of defining the same smooth gauge condition over all space-time. There is no such topological obstruction on the lattice since all gauge conditions are necessarily discontinuous.[8] Nevertheless, F_L is a very complicated function in a space of many dimensions and it is hard to see why it should not have many local maxima. The numerical results (Fig. 2) suggest that F_L can become quite flat in some directions on the way to the maximum. We have looked for Gribov copies on small (2^4) lattices by applying the gauge fixing algorithm to configurations related by a random gauge transformation. In all cases we found, by studying the trace of each link, that the final configurations differed only by a global gauge transformation when θ [Eq. (3.6)] was reduced to 0.0 within machine precision. Since the different configurations take a different route to the final one under the gauge fixing algorithm, the gauge fixing cannot be complete if θ is simply reduced to a small nonzero value. This point makes Landau gauge on its own rather difficult to use and will be discussed further in Sec. IV.

When studying lattice QCD above the deconfinement phase transition with no fermions it may be necessary to change Eqs. (3.1) and (3.6) to be Z_3 invariant. This will ensure that the gauge has similar properties in the three different phases of the theory. A suitable choice for F_L might be

$$F_L=\frac{1}{N_C}\frac{1}{4V}\sum_{\mu,x}\mathrm{Tr}[U_\mu(x)]\,\mathrm{Tr}[U_\mu^\dagger(x)]\ . \tag{3.12}$$

Even when this quantity is maximized, the gauge is fixed only up to a local transformation by elements of Z_3. This will usually be sufficient, however, since elements of Z_3 commute with all the link fields.

IV. DISCUSSION OF LATTICE GAUGE FIXING

One of the pleasing aspects of the Wilson formulation of gauge theories on a lattice is that the gauge fields take values in a compact space so that the functional integral over these fields is finite. The Feynman path integral can then be calculated numerically without fixing the gauge.

There are many situations, however, where it is helpful to have configurations of link fields with certain properties that result from having fixed a particular gauge. Measurements of gauge-invariant loop operators become simple to implement numerically, for example, when some of the links in the loop are gauge fixed to the identity. It also becomes possible to measure gauge-noninvariant quantities, such as the gluon propagator, and give some meaning to them.[9] If the spurious gauge degrees of freedom are all removed then extended operators which cover more than one site become well defined without the numerical difficulty of putting a string of link fields between the sites. This would apply to products of fermion fields on different sites that are used to measure hadron wave functions.[10] In a suitable gauge, such as Landau gauge, the wave functions would be well behaved and easy to measure. These are all examples of the use of gauge fixing to cut the computational cost of making certain measurements in a numerical simulation. We have been primarily concerned, on the other hand, with the use of gauge fixing in algorithms that modify the usual time evolution of the numerical simulation.

One of the best frameworks for discussing the way in which a numerical simulation of a field theory evolves in computer time is one in which the consecutive members of the ensemble of field configurations are generated using a discretized Langevin equation. The link fields at Langevin step $n+1$ are calculated from those at step n according to

$$U_\mu^{(n+1)}(x)=e^{if_jT^j}U_\mu^{(n)}(x)\ . \tag{4.1}$$

For each link, the force term of the Langevin equation takes the form

$$f_j=\epsilon\partial_jS[U]+\sqrt{\epsilon}\eta_j\ , \tag{4.2}$$

where ∂_jS is a derivative of the action along the group manifold with respect to that link, ϵ is the Langevin time step and η is a noise term drawn independently from a Gaussian distribution for each link.

The updating algorithm for the gauge fields is rather like an optimization algorithm with noise. It suffers from critical slowing down as we take the continuum limit ($a\to 0$) on a lattice of fixed physical volume. This critical slowing down will be present for all local updating schemes such as the Metropolis algorithm, heat bath, etc. The Langevin algorithm has the useful feature that, by making a nonlocal update, Fourier acceleration can alleviate the problem and enable decorrelated measurements to be made with less computer time. This will be discussed more fully in a forthcoming paper.[4] Here we simply note that it is necessary to fix to a suitable gauge for Fourier acceleration of a non-Abelian gauge theory.

Another algorithm useful in lattice gauge theory simulations is that of matrix inversion. This is another problem with critical slowing down and we shall describe elsewhere the application of Fourier acceleration to the conjugate-gradient algorithm for Wilson fermions.[3] Again we require that the link fields be in a suitable gauge.

Both the algorithm for the inversion of the fermion matrix and that for the updating of the gauge fields are controlled by matrices which are not gauge invariant. We therefore have to fix to a gauge in which their form has the best momentum-space structure for Fourier acceleration. This seems to be a gauge in which the average trace link [F_L of Eq. (3.1)] is close to 1 and θ is close to 0. Then the magnitude of the high-momentum components of the gauge field will be small, as will interaction terms which couple fields of widely different momenta in the fermion matrix or the updating force term. We have tested various gauges for their compatibility with Fourier acceleration. We shall describe below the gauge which we have found to work best and which we call the "AL gauge." It is a combination of an axial-type gauge and a Landau-type gauge.

First let us describe how to generate an ensemble of gauge-fixed configurations in a simulation of a lattice gauge theory. There are two alternatives. The first is to

update the link fields in such a way as to maintain the gauge condition (or at least to break the gauge invariance). The second is to extend the updating process to include two steps, an update of all the link fields in the usual manner followed by a step in which the fields are gauge transformed into the appropriate gauge.

The first alternative has been studied in the case of axial gauges[11–13] (see the Appendix). Here it is easy to maintain the gauge condition by simply not updating the links on the maximal tree. Unfortunately it was found that, even though some time was saved on each updating step, the simulation was slowed down and decorrelation times became very long. The basic reason for this is that when only some links are allowed to fluctuate the phase space is explored less efficiently. This is a case where the use of gauge fixing has affected the time evolution of the numerical simulation adversely.

The second method, and the one that we use, involves gauge fixing the fields in between the usual updating steps. In this way the configurations obtained are gauge transformations of those that would have been obtained without gauge fixing, and the time evolution of the numerical simulation will not be affected by this method of gauge fixing.

It is also important to ensure the gauge covariance of the algorithm. This requires that gauge-equivalent configurations be updated by the algorithm so that their gauge equivalence is maintained. Physical quantities measured on the two configurations will then remain identical, step by step, as they must. For a local updating process, such as that in the Metropolis algorithm or the Langevin algorithm with no Fourier acceleration, gauge transformations commute with updating steps and gauge covariance is easy to show. In the local Langevin algorithm it follows because

$$e^{i[f_j T^j]^g} U_\mu^g(x) = e^{iG(x) f_j T^j G^\dagger(x)} G(x) U_\mu(x) G^\dagger(x+\hat{\mu}) = G(x) e^{i f_j T^j} U_\mu(x) G^\dagger(x+\hat{\mu}) \,. \quad (4.3)$$

When Fourier acceleration is applied, with its nonlocal force term, gauge covariance can still be maintained if the updating process includes a complete gauge fixing. Then all gauge-equivalent configurations become the same under the gauge fixing and will automatically be updated identically. As discussed in previous sections and in the Appendix, a complete gauge fixing is provided by an axial gauge or (probably, given enough iterations) by Landau gauge on its own. It will also be true of an axial gauge fixing followed by gauge transformations which would not on their own provide a complete gauge fixing. We use this fact to define the AL gauge which is an axial gauge fixing followed by a given number of hits of the algorithm described in Sec. III for fixing to Landau gauge. This is a well-defined gauge in the sense that the gauge-fixing condition can be written as a relation between links on the lattice. The relation involves the gauge transformation matrices on the sites and these are simply an ordered product of those for the axial gauge followed by each hit of the Landau gauge-fixing algorithm:

$$G(x) = G_{L(n)}[U^{L(n-1)}] \cdots G_{L(2)}[U^{L(1)}] \times G_{L(1)}[U^{\text{axial}}] G_{\text{axial}}[U] \,. \quad (4.4)$$

This gauge will have similar properties to Landau gauge and yet will be much simpler and faster to implement. It will have a value for θ [Eq. (3.5)] which is small, although not zero (in fact it will fluctuate from configuration to configuration). We find, when working on an 8^4 lattice at $b=5.8$, that 5 hits of the Landau gauge-mixing algorithm is sufficient to give Fourier acceleration of the fermion matrix inversion when the axial gauge that is used is the blocked one discussed in the Appendix. If the axial gauge used is the lattice temporal gauge ($A^0=0$) then 10 hits of the Landau gauge-fixing algorithm are required. This corresponds to a value for θ of about 0.5 (the value without gauge fixing is 14) and a value for F_L of about 0.77.

An axial gauge on its own did not produce good results in a Fourier accelerated updating algorithm. For the $A^0=0$ gauge this appears to be because there are large fluctuations in the field for small values of k^0 even when $\mathbf{k}$ is large, directly related to $1/(k^0)^2$ singularities in the continuum axial gauge propagator. On the lattice this translates into the fact that the length of string along the maximal tree joining two sites which are nearest neighbors in a direction perpendicular to the t axis is of order L, the length of the lattice. This was the motivation for trying the blocked axial gauge where the length of the longest string along the tree grows only as $\ln(L)$. This gauge performed considerably better than the temporal gauge on an 8^4 lattice but still did not allow for Fourier acceleration. It had a value for F_L of 0.43 compared to 0.31 for the $A^0=0$ gauge. Perhaps the blocked axial gauge will be useful on its own on larger lattices but in the meantime we use it as a good first step in fixing to AL gauge.

V. CONCLUSIONS

We have described the technique of Fourier acceleration and its application to problems in numerical optimization. One particular application that we have discussed is the gauge fixing to Landau gauge of link fields on a lattice. Landau gauge has the useful properties that it is translationally invariant and "smooth," in the sense that high-momentum fluctuations in the field are small. This makes it the gauge of choice where one is needed for measurements.

Unfortunately, algorithms to achieve this gauge fixing suffer from critical slowing down, so they become very costly on large lattices. We have demonstrated that critical slowing down can be virtually eliminated from this problem by the use of Fourier acceleration. The number of iterations of the algorithm required becomes independent of the volume. Our tests with the steepest descents algorithm on an 8^4 lattice of SU(3) links at $\beta=5.8$ show that the computer time required is reduced by a factor of 5 when Fourier acceleration is used. As the volume is increased this gain will improve.

Of course, the naive steepest-descents algorithm is not very efficient and better optimization methods, such as

conjugate gradient, can be considered. These will suffer from critical slowing down, however, and will need the application of Fourier acceleration to make them viable algorithms on large lattices. This means that the algorithm must be capable of translation into momentum space; i.e., it must calculate $G(x)$ everywhere simultaneously. It is hard to see how Fourier acceleration could be used with algorithms which optimize at a single site and then move on, such as the Gauss-Seidel algorithm. We have not investigated more sophisticated optimization techniques for Landau gauge fixing because we need, for our purposes, only a few hits of the accelerated steepest-descents algorithm and that is very fast.

Our interest in gauge fixing has arisen because it is a prequisite for the Fourier acceleration of other algorithms necessary for simulations of lattice gauge theories. These are matrix inversion and the generation of an appropriate ensemble of gauge fields. We find that these algorithms can be accelerated successfully when the link fields are in AL gauge, defined as axial gauge followed by 5–10 hits of the accelerated Landau gauge-fixing algorithm. This is a fast gauge to implement, gives a complete gauge fixing and produces link fields with an acceptable structure in momentum space to enable greatly improved efficiency in realistic simulations of lattice QCD.

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APPENDIX: AXIAL GAUGE FIXING ON THE LATTICE

In axial gauges $(V-1)$ links are gauge transformed to the unit matrix. These links form a maximal tree on the lattice which has no closed loops and many shapes of this tree are possible.

The lattice temporal gauge, $A^0=0$, has the comblike structure illustrated for a 2^3 lattice in Fig. 4(a). The gauge transformation matrices which will fix to this gauge in one step are made up of products of links joining the site that they sit on, x, to the origin along the tree:

$$G(x,y,z,t)=U_x(0,0,0,0)\cdots U_y(x,0,0,0)\cdots \times U_z(x,y,0,0)\cdots U_t(x,y,z,t-1)\ . \quad \text{(A1)}$$

This is clearly a complete gauge fixing—all local gauge degrees of freedom having been removed. Notice that $G(x)$ transforms under a gauge transformation on the original U fields, such as

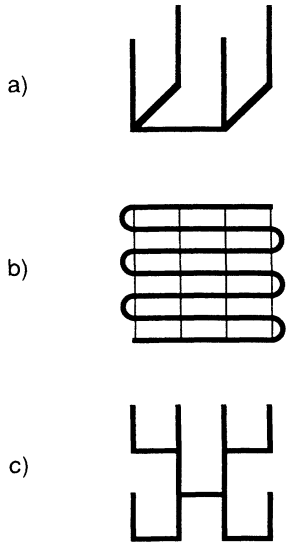

FIG. 4. (a) The maximal tree for the $A^0=0$ gauge, drawn for a 2^3 lattice. (b) The maximal tree for the $A^1=0$ gauge on a 4^2 lattice with skew-periodic boundary conditions on the gauge field. (c) The maximal tree for the blocked axial gauge, illustrated for a 4^2 lattice.

$$G(x)\to g(0)G(x)g^\dagger(x)$$
$$\text{when } U_\mu(x)\to g(x)U_\mu(x)g^\dagger(x+\mu)\ , \quad \text{(A2)}$$

so that $G(x)U_\mu(x)G^\dagger(x+\mu)$ is invariant up to a global gauge transformation.

Other shapes for the maximal tree can be imagined. The $A^1=0$ gauge on a lattice with skew-periodic boundary conditions has a snakelike structure illustrated in Fig. 4(b). Both this and the $A^0=0$ gauge have the disadvantage of breaking translational invariance of the lattice in a particular direction so that momentum is not conserved in interactions between particles and the gauge field. For the snake gauge it is a very small effect since only one site in the x direction looks different from the rest.

A numerical problem with fixing axial gauges on large lattices is that any roundoff error in the U matrices that makes them nonunitary will be amplified by the process of multiplying long strings of them together. The U matrices should be reunitarized before axial gauge fixing.

There exist other axial gauges where the maximal tree is distributed throughout the lattice, for example, the random axial gauge.[12] We use a gauge which we call the blocked axial gauge in which the maximal tree is built up from smaller 2^4 units in an iterative way. It is most simple to visualize for lattices whose sides have length a power of 2 and is illustrated for a two-dimensional lattice in Fig. 4(c).

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