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Ground-state projection multigrid for propagators in four-dimensional SU(2) gauge fields*

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The ground-state projection multigrid method is studied for computations of slowly decaying bosonic propagators in four-dimensional SU(2) lattice gauge theory. The defining eigenvalue equation for the restriction operator C is solved exactly. With the Galerkin choice $\mathcal{A} = C^*$ for the interpolation operator, the critical exponent z is not reduced in nontrivial gauge fields. Nevertheless, a considerable speedup is obtained compared to conventional relaxation, and the conjugate gradient algorithm is outperformed. Simulations with an "optimal" interpolation kernel $\mathcal{A}$ eliminate critical slowing down for any value of the gauge coupling. This proves that ground-state projection is a good choice of C (i.e., of the blockspin).

In Monte Carlo simulations of lattice gauge theories with fermions the gauge field dependent fermion propagator S needs to be computed anew for each new gauge field configuration. Therefore it is important to have an efficient method to do so. More precisely one needs $u = Sf$, where f are given functions. The conjugate gradient (CG) algorithm is state of the art. Great hopes to do better are attached to the multigrid (MG) method [1–6]. The ground-state projection method is particularly attractive. There, the averaging operator C from a grid to the next coarser grid is a projector on the ground state of a local hamiltonian. Initial results in 2D U(1) [3,4] and (approximate ground-state projections) in 2D and 4D U(1) and 2D SU(2) gauge fields [3,5] are encouraging, but applications in 4D non-abelian gauge fields remain a challenge because of the difficulty of finding the projector.

Here we present the first ground-state projection MG computation of a gauge covariant propagator in 4D, for SU(2) gauge fields. We consider the bosonic propagator $(-\Delta + m^2)^{-1}$, where Δ is the gauge covariant lattice laplacian. The MG method is of interest near criticality, i.e., for slowly decaying propagators. For nontrivial gauge fields we enforce slow decay by choosing m^2 negative and very close to the negative of the lowest eigenvalue $-m_{\rm cr}^2$ of $-\Delta$.

The method used for finding the projector C depends essentially on the absence of degeneracies of the eigenvalues of the local hamiltonian (modulo the intrinsic two-fold degeneracy discussed below). This nondegeneracy condition can also be fulfilled for staggered fermions, provided the averaging is chosen such that it leads to staggered fermions on the coarse lattice again (unlike in ref. [4]). However, staggered fermions have special problems associated with flavor symmetry breaking. Therefore it seemed worthwhile to do a bosonic computation first.

We divide the original hypercubic lattice Λ of lattice spacing a (set = 1) into hypercubes ("blocks") x of $L_{\rm b}^4$ sites $z \in \Lambda$, with $L_{\rm b} = 3$. We identify each such hypercube x with the site $\hat{x}$ at its center. These sites $\hat{x}$ form the first block lattice Λ^1 with lattice spacing $L_{\rm b}a$, and so on. The averaging C is supposed to map two-component functions on Λ into two-component functions on Λ^1. Its kernel $C(x, z)$ is a 2×2 matrix. We demand that $C(x, z) = 0$ unless $z \in x$. Mack's version of the projective MG method will be used. It is briefly reviewed below and described in some detail in refs. [7,8]. The "local hamiltonian" on hypercube x is $-\Delta_{N,x}$. This is a discretized version of the gauge covariant laplacian with Neumann boundary conditions on the boundary of

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hypercube x. Explicitly

$$(\Delta_{N,x} f)(z) = \sum_{\substack{w \text{ n.n. } z, \\ w \in x}} [U(z,w) f(w) - f(z)] \quad (1)$$

for $z \in x$, and 0 otherwise. Summation runs over the nearest neighbors w of z which are in the same hypercube x, $U(z,w) \in \mathrm{SU}(2)$ is the lattice gauge field attached to link (z,w).

We introduce the notation $C^*(z,x) = C(x,z)^\dagger$ ($\dagger$ is the adjoint of a 2×2 matrix). For each x the averaging kernel $C(x,z)$ is determined as a solution of the gauge covariant eigenvalue equation

$$(-\Delta_{N,x} C^*)(z,x) = \lambda_0(x)\, C^*(z,x). \quad (2)$$

The laplacian acts on z, and $\lambda_0(x)$ is the lowest eigenvalue of the positive (semi-)definite operator $-\Delta_{N,x}$. When eq. (2) is regarded as an equation for a two-component vector in place of a matrix, then it has two degenerate solutions, for any gauge field. To see this suppose that $(c_{11}, c_{12}, c_{21}, c_{22}, \ldots, c_{V1}, c_{V2})^{\mathrm{T}}$, $V = L_{\mathrm{b}}^{\mathrm{d}}$, is an eigenvector of $-\Delta_{N,x}$ corresponding to an eigenvalue λ. By using the fact that the elements of (a multiple of) an SU(2) matrix $(U_{ij})_{i,j=1,2}$ fulfill $U_{21} = -\overline{U_{12}}$, $U_{22} = \overline{U_{11}}$, one proves that $(-\overline{c_{12}}, \overline{c_{11}}, -\overline{c_{22}}, \overline{c_{21}}, \ldots, -\overline{c_{V2}}, \overline{c_{V1}})^{\mathrm{T}}$ is also an eigenvector of $-\Delta_{N,x}$ with the same eigenvalue λ. The two independent two-component solutions may be combined into a 2×2 matrix $C^*(z,x)$ The freedom of taking linear combinations reflects itself in the freedom of taking $C^*(z,x) \to C^*(z,x)\Omega(x)$, where $\Omega(x)$ is an arbitrary 2×2 matrix. This freedom is eliminated by imposing the normalization condition

$$CC^* = I,$$

$$\text{i.e., } \sum_z C(x,z) C^*(z,y) = L_{\mathrm{b}}^{-4} \delta_{x,y} I \quad (3)$$

and

$$C(x,\hat{x}) = r(x)\, I, \quad \text{with } r(x) > 0 \text{ real}. \quad (4)$$

The second condition ensures that the averaged field $\Phi(x) = (C\phi)(x)$ on Λ^1 transforms under gauge transformations like the field ϕ on Λ at block center $\hat{x}$. An efficient algorithm for solving eq. (2) was described by the author in ref. [7], and was used in this work.

In the MG approach one introduces a sequence of lattices $\Lambda = \Lambda^0, \Lambda^1, \Lambda^2, \ldots$ of increasing lattice spacing a_i, viz. $a_{i+1} = L_{\mathrm{b}} a_i$ with $a_0 = a$. We wish to solve an inhomogenous linear equation

$$\mathrm{D}_0 u_0 = f_0 \quad (5)$$

on the fundamental lattice $\Lambda = \Lambda^0$, for given f_0. In our case, $\mathrm{D}_0 = -\Delta + m^2$. After some relaxation sweeps on Λ^0 one gets an approximation $\tilde{u}_0$ to u_0 which differs from the exact solution by an error $e_0 = u_0 - \tilde{u}_0$. The fundamental idea of the MG to the solution of partial differential (or difference) equations [9] is that the error e_0 should become smooth very fast, although it may become small very slowly because of critical slowing down (CSD). The error satisfies the equation

$$\mathrm{D}_0 e_0 = r_0 \quad (6)$$

which involves the residual $r_0 = f_0 - \mathrm{D}_0 \tilde{u}_0$. If e_0 is smooth, it is determined to a very good accuracy by a function e_1 on the next coarser lattice Λ^1, and can be represented in the form

$$e_0 = \mathcal{A} e_1 \quad (7)$$

with an interpolation map $\mathcal{A}$ which should be so chosen that it maps functions on Λ^1 into smooth functions on Λ^0. Conversely, e_1 can be obtained from e_0 with the help of an averaging map C which satisfies

$$C\mathcal{A} = I. \quad (8)$$

It follows that $e_1 = Ce_0$. Inserting eq. (7) into eq. (6) and acting on the result with C, we see that e_1 will satisfy the equation

$$\mathrm{D}_1 e_1 = r_1 \quad (9)$$

with

$$\mathrm{D}_1 = C\mathrm{D}_0\mathcal{A}, \quad r_1 = Cr_0. \quad (10)$$

The problem has been reduced to an equation on the coarser lattice. If there is still too much CSD at this level, one may repeat the procedure, going to coarser and coarser lattices. Instead, eq. (9) on the coarser lattice was solved exactly by CG. This suffices to test the power of the MG method. In 4D with $L_{\mathrm{b}} = 3$, Λ^1 has 81 times fewer points than Λ^0.

In bosonic gauge theories, the natural definition of smoothness of a function e on Λ^0 is that its covariant derivative $\nabla_\mu e$ should be small:

$$||\nabla_\mu e||^2 \equiv (\nabla_\mu e, \nabla_\mu e) = (e, -\Delta e) \ll (e, e). \quad (11)$$

Except for a pure gauge, the lowest eigenvalue of $-\Delta$ is strictly positive. It can be regarded as a measure of disorder of the gauge field. Thus, in a disordered gauge field there is a limit to how smooth a function can be.

Given the averaging kernel C, there exists an ideal choice of the interpolation kernel $\mathcal{A}$. It is determined as follows. For every function ("block-spin") Φ on Λ^1, $\phi = \mathcal{A}\Phi$ minimizes the action $\mathcal{H} = (\phi, (-\Delta + m^2)\phi)$ subject to the constraint $C\phi = \Phi$. With this choice of $\mathcal{A}$, D_1 is guaranteed to be self-adjoint. A good "choice of block-spin", i.e., of C, is characterized by the fact that the ideal kernel $\mathcal{A}(z,x)$ ($z \in \Lambda^0$, $x \in \Lambda^1$) associated with it has good locality properties. This means that $\mathcal{A}(z,x)$ is big for $z \in x$, and decays exponentially in $|z - \hat{x}|$ with decay length 1 block lattice spacing a_1. Computations of the ideal kernel $\mathcal{A}$ were done and it was verified that the choice (2) of C is a good choice of blockspin in this sense, and that the exact D_1 of eq. (10) is to a good approximation of the same nearest neighbor form as $D_0 = -\Delta + m^2$. If x and y are nearest neighbors then $D_1(x,y) = \sum_z C(x,z) D_0 \mathcal{A}(z,y) = C D_0 \mathcal{A}(x,y)$ can be regarded as a dielectric lattice gauge field [10] on the link (x,y) of Λ^1. It is equal to an SU(2) lattice gauge field multiplied with a fluctuating positive real factor ("fluctuating length").

The interpolated solution $e_0 = \mathcal{A} e_1$ of eq. (9) is supposed to be added to the approximate solution $\tilde{u}_0$ of eq. (6) to obtain the true solution u_0. With the ideal choice of $\mathcal{A}$, there is complete decoupling between layers[#1]. But the exponential tails of the ideal $\mathcal{A}$ make it impractical for actual simulations, and too costly to compute over and over again.

If we approximate $\mathcal{A}$, maintaining $C\mathcal{A} = I$ and retaining the exact D_1 (for the moment), then the interpolated solution $e_0 = \mathcal{A} e_1$ of eq. (9) will yield the right correction of the low frequency part of $\tilde{u}_0$, but it re-introduces an error in the high frequency part. To eliminate this error, one has to go back to Λ^0 and do iterations there again. In other words, the whole two-grid cycle has to be iterated. We adopt the Galerkin choice (variational coarsening, VC)

$$\mathcal{A} = C^*. \quad (12)$$

Without knowing the exact kernel $\mathcal{A}$, one cannot compute the exact "effective difference operator" D_1. Knowing that D_1 is approximately of nearest neighbor form as described above, one can try to approximate it. The choice

$$D_1 = \delta^{-1} C D_0 C^* \quad (13)$$

yields another dielectric lattice gauge field $D_1(x,y)$ which also has the right gauge covariance properties. Its fluctuating length can be adjusted to fluctuate around the "right" value (of the exact $D_1(x,y)$) by adjusting the real parameter δ. One could think of adjusting also m^2 in D_1, but it turned out that this leads to no more than a $\sim 5\%$ acceleration of convergence.

The exact kernel $\mathcal{A}$ can be used to carry out systematic investigations of the question where one buys what error and how it affects convergence speed. Such studies were also done and will be discussed below. First we report on the performance of a scheme based on the choice (2)–(4), (12), (13).

To get good performance it is essential to choose an efficient iteration scheme on Λ^0. We used damped Jacobi iteration and successive over-relaxation (SOR) with an adjustable relaxation parameter ω. (The notation for ω is standard, see e.g. ref. [11].) This includes Gauss–Seidel relaxation as a special case ($\omega = 1$).

Numerical work was done on 9^4 and 18^4 lattices Λ with SU(2) gauge fields equilibrated with the Wilson action at various values of β. We compare damped Jacobi iteration on a single layer (Jac), SOR-iteration on a single layer (SOR), conjugate gradient on a single layer (CG) and two versions of

[#1] This means the following: We may regard eq. (5) as an eq. (5′) for the high frequency part $u_0^h = u_0 - \mathcal{A} C u_0$ of u_0. This equation is noncritical and therefore iteration of (5′) should converge quickly to yield u_0^h accurately. If it has converged in this sense, then addition of the interpolated solution of eq. (9) produces the true solution u_0 of (5). There is no need to repeat the whole procedure.

Table 1
MG with VC: optimum values of δ and ω in a 4D pure gauge ($m_{cr}^2 = 0$) and demonstration of elimination of CSD.

Algorithm and lattice size	Optimal δ	Optimal ω	Relaxation time τ for m^2 =			
			1.0	0.1	0.01	$10^{-3}, \ldots, 10^{-10}$
MG Jacobi on 9^4	1.8	0.96	3.6	6.4	7.1	7.2
MG Jacobi on 18^4	1.8	0.94	4.0	6.4	6.9	7.0
MG SOR on 18^4	1.7	1.09	2.3	2.5	2.8	2.9

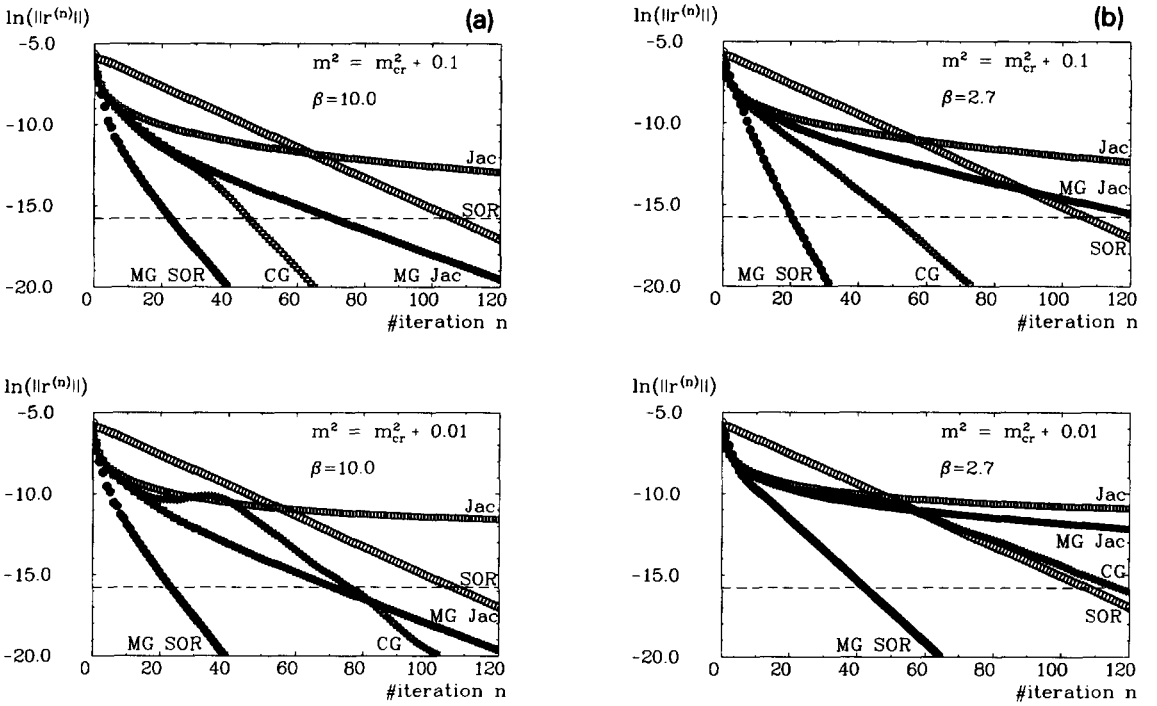

Fig. 1. Convergence on an 18^4 lattice in quenched SU(2) gauge fields at (a) $\beta = 10.0$, and (b) $\beta = 2.7$, with $m_{cr}^2 = -0.1533739$, respectively -0.7554339. (MG with VC.)

two-grid cycles, MG Jac and MG SOR with checkerboard updating. One iteration of the two-grid cycle consists of exact solution of the residual equation on the 3^4 respectively 6^4 block lattice Λ^1 by CG, followed by one sweep through the lattice Λ^0 using either Jacobi or SOR. The computational work done in one iteration of all schemes is comparable. The propagator was computed, i.e., f_0 is a Kronecker δ.

Relaxation times τ (in number of iterations) were determined as follows. Let $r^{(i)}$ be the residual on Λ^0 after the ith iteration. The RMS residuals $||r^{(i)}|| \equiv \{|\Lambda^0|^{-1} \sum_{z\in\Lambda^0} \frac{1}{2}\mathrm{Tr}\,[r^{(i)}(z)^\dagger r^{(i)}(z)]\}^{1/2}$ were computed, and τ was determined from an exponential fit after $||r^{(i+1)}||/||r^{(i)}||$ has become constant with an accuracy of better than 10^{-4} for at least 50 iterations.

For pure gauges, complete elimination of CSD was observed in the MG iterations, and CG which has CSD was clearly outperformed. Results are in table 1. The results were also checked for gauge covariance.

For nontrivial gauge fields the lowest eigenvalue $-m_{cr}^2 > 0$ of $-\Delta$ was first determined by inverse iteration to an accuracy of 10^{-7} or better (see data in fig. 2). Propagators $(-\Delta + m^2)^{-1}$ were computed for

values of m^2 close to criticality, $m^2 = m_{cr}^2 + \Delta m^2$, $\Delta m^2 = 1, 0.1, 0.01, 0.001, \ldots, 10^{-7}$. Optimum values of ω and δ are (i) $\beta = 10.0$: $\delta \sim 2.3$, $\omega \sim 0.99, 0.96, 1.25$ for MG Jacobi on a 9^4, on an 18^4, and for MG SOR on an 18^4 lattice respectively; (ii) $\beta = 2.7$: $\delta \sim 2.8$, $\omega \sim 0.99, 0.99, 1.51$ for algorithms as above. These values were determined at $\Delta m^2 = 0.01$ and retained for all values of m^2. For pure gauges, performance of the MG schemes depends little on δ, but for disordered gauge fields, the relaxation time decreased with increasing δ up to a maximum value where the MG algorithms start to diverge suddenly.

In fig. 1 the approach to convergence of the various algorithms is compared for two nonpure gauge field configurations ($\beta = 10.0$ and $\beta = 2.7$) for values $\Delta m^2 = 0.1, 0.01$, with ω, δ in MG as given above, $\omega = 0.99$ in Jac, $\omega = 1.91$ in SOR. The initial guess for the propagator is zero in case of CG and $\delta_{z,0}\,\omega/(8 + m^2)$ for the relaxation algorithms. In the literature, convergence is considered achieved when the natural logarithm of the RMS residual has gone down by 10 (dashed line in fig. 1). It is seen that MG SOR outperforms CG.

Smaller values of Δm^2 may seem to be of no practical importance because the correlation length determined by the propagator becomes comparable to or larger than the lattice extension, and finite size effects are important. But it is nevertheless important to study very small Δm^2 in order to understand the operation and limits of the MG algorithms.

In fig. 2 the relaxation time for various algorithms is shown as a function of Δm^2, at $\beta = 2.7$. One sees that CSD is not eliminated in the MG modes. The relaxation time behaves like $\tau \propto (\Delta m^2)^{-z/2}$ with $z = 2$ both for MG Jac and MG SOR[#2]. (CG has no well defined τ.) At $\beta = 10.0$ the same qualitative behavior was found as in fig. 2. Computations at other β's down to 2.2 were also done. Surprisingly it was found that the value of Δm^2 at which CSD sets in (i.e., τ starts to increase) depends little on β. This contradicts the scaling hypothesis of ref. [5]. Basically the only dependence on β was found

[#2] τ's for relaxations on a single grid are known functions of m_{cr}^2, and agree extremely well with with our numerical results. This will be discussed in more detail elsewhere.

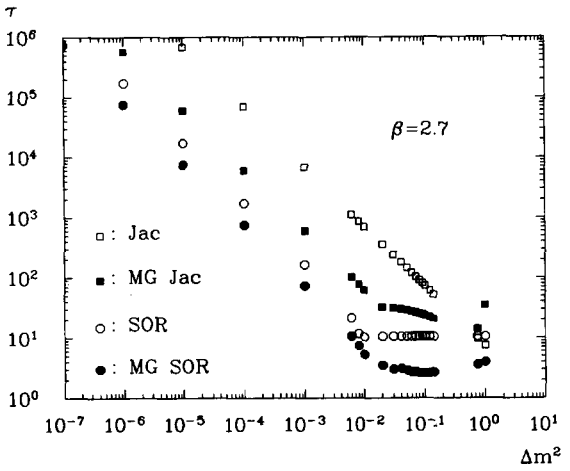

Fig. 2. Relaxation times τ (in comparable work units) of iterative algorithms on an 18^4 lattice in a quenched SU(2) gauge field at $\beta = 2.7$, with $m_{cr}^2 = -0.7554339$. (MG with VC.)

for the constant of proportionality in the scaling relation of τ. Compared with $\beta = 2.7$, its value is nearly doubled for $\beta = 2.2$, and roughly reduced by a factor of 3 at $\beta = 10.0$.

A tentative interpretation of the permanence of CSD might be as follows: m_{cr}^2 is a natural gauge invariant measure of smoothness (see above). For $\beta \leqslant 10$ the lowest eigenvalue $-m_{cr}^2$ of $-\Delta$ appears to be too large to consider any function on Λ^0 as smooth. Therefore the basic hypothesis of the MG method, namely smoothness of the slow modes, is not fulfilled, and therefore one cannot expect MG to work in an optimal fashion. There would be no problem if one had restricted attention to propagators $(-\Delta + m^2)^{-1}$ with $m^2 \geqslant 0$. This propagator is critical only when $-\Delta$ has a very low eigenvalue, and then smooth functions exist.

One might believe that basically one is paying the prize for having introduced criticality artificially into a frustrated system. However, investigations with Mack's optimal interpolation kernel $\mathcal{A}$ [12,8] showed that this is not the case.

The optimal $\mathcal{A}$ was computed for gauge fields on 9^4 lattices at $\beta = \infty$, 2.7, 2.5, 2.2, 1.8, 0. $\mathcal{A}$ is the solution of the equation

$$([-\Delta + m_{cr}^2 + \kappa\, C^* C]\mathcal{A})(z,y) = \kappa\, C^*(z,y) \quad (14)$$

for large κ. This $\mathcal{A}(z,y)$ is not translational invari-

Table 2
Results of the idealized MG algorithm with lexicographic SOR on 9^4 lattices Λ^0.

β	m^2_{cr}	optimal ω	τ for $\Delta m^2 \leqslant 10^{-3}$
∞	0	1.27	1.6
2.7	−0.8210607	1.38	1.9
2.5	−0.9477085	1.40	1.9
2.2	−1.2218471	1.45	1.9
1.8	−1.7567164	1.57	2.5
0	−2.7480401	1.69	5.2

ant (except for $U \equiv I$) and has support on all 9^4 sites z of the fine lattice, for all 3^4 sites y of the block lattice. The use of this kernel for production runs is impractical, but it is important to answer questions of principle. (These investigations had to be done on small 9^4 lattices because of storage space requirements.)

It turned out that CSD is completely eliminated at any value of β when $D_1 = CD_0\mathcal{A}$ *and* e_1 is interpolated by $\mathcal{A}$. Results are in table 2. Relaxation times in the optimal MG scheme are less dependend on ω than in VC. Also, no damping parameter δ is required. The fact that CSD is completely eliminated in the idealized MG algorithm proves that ground-state projection is a good choice of C (i.e., of a smooth blockspin of the low frequency components) in gauge theories.

Finally, it is interesting to note that CSD is not eliminated in nontrivial gauge fields when not all ingredients are optimal. Choosing either $D_1 = \delta^{-1}CD_0\mathcal{A}$ but using C^* instead of $\mathcal{A}$ for interpolation, or approximating $D_1 = \delta^{-1}CD_0C^*$ but retaining $\mathcal{A}$ for interpolation, both fail to eliminate CSD at finite β. This is unlike the case $\beta = \infty$, where also these two modifications of the idealized algorithm succeed in fighting CSD. When no gauge fields are present, the lowest mode of $-\Delta$ is a constant. In this case the simple variational MG scheme is successful, because then C^* interpolates the lowest mode of $-\Delta$ correctly. The same is true for the optimal $\mathcal{A}$, since it fulfills $(L_b a)^4 \sum_{y\in\Lambda^1} \mathcal{A}(z,y) = 1$ for all $z \in \Lambda^0$. In the trivial case $U = I$ the interpolation of a constant function on Λ^1 with $\mathcal{A}$ is unnecessarily complex, because there are nonvanishing contributions from all $y \in \Lambda^1$. However, the above results show that indeed more complicated choices of D_1 *and* of the interpolation map $\mathcal{A}$ are necessary to obtain $z = 0$ in bosonic gauge theories.

With staggered fermions the situation is different from the bosonic one in principle. The gauge covariant Dirac operator $\not{\nabla}$ has an eigenvalue close to zero in disordered gauge fields, and there exist therefore functions which are smooth in the sense that $||\not{\nabla}e||^2$ is small. Unfortunately, it is costly in memory and storage space to try to exploit this – see the discussion in ref. [8]. Therefore the result of this paper that schemes based on "laplacian smoothness" (11) work well enough suggests that one may not have to pay this prize.

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