
Adaptive Smoothed Aggregation in Lattice QCD

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Summary. The linear systems arising in lattice quantum chromodynamics (QCD) pose significant challenges for traditional iterative solvers. The Dirac operator associated with these systems is nearly singular, indicating the need for efficient preconditioners. Multilevel preconditioners cannot, however, be easily constructed for these systems because the Dirac operator has multiple locally distinct near-kernel components (the so-called slow-to-converge error components of relaxation) that are generally both oscillatory and not known a priori. This paper presents heuristic arguments and numerical results demonstrating that the recently developed adaptive smoothed aggregation (α SA) [BFM⁺04] methodology can be used to overcome the challenges posed by these systems.

1 Introduction

In the field of particle physics, the “Standard” model accounts for the interactions between the elementary particles that make up matter. The Standard model is completely described by two theories: the Electroweak theory for weak interactions, and the widely accepted QCD theory for strong interactions. The interactions between these constituents of matter are well understood for Electroweak theory, where they can be analyzed analytically using perturbation theory. For strong interactions between fermions (quarks), the coupling forces are so strong that a perturbation theory analysis becomes

increasingly complex and ultimately breaks down. In the early 1970's, Wilson proposed simulating these strong interactions numerically using Lattice Gauge Theory (LGT), effectively discretizing QCD [Crtz82]. LGT is now the primary means for modeling such strong interactions. However, a major obstacle remains: current LGT simulations require enormous computations that become prohibitively expensive for physically interesting choices of parameters (e.g., quark mass and temperature of the physical system), even on today's supercomputers. Hence, the understanding of strong interactions is still very limited.

The majority of the computations in these numerical simulations is dedicated to solving the linear Dirac systems arising from discretization of a coupled system of PDEs on a four-dimensional space-time lattice. This is due to the fact that, in current state-of-the-art simulations, the solvers used for these systems are limited to Krylov methods with preconditioners that are suboptimal for interesting choices of the physical parameters [Bra92, BER⁺91]. Developing an appropriate preconditioner for these systems has been a topic of intense research for many years. In the 1990's, various multigrid approaches were explored [Bra92, BER⁺91]. More recently, in [Lu04], the use of an alternating Schwarz preconditioner was studied.

This paper considers a simplified 2D Schwinger model exhibiting similar challenges to those of the four-dimensional problem of interest. We explore the use of an adaptive smoothed aggregation [BFM⁺04] iterative solver for these systems. The remaining sections are organized as follows. In §2, we present the 2D Hermitian Dirac-Wilson operator. In §3, we discuss the properties of the 2D operator. Numerical results demonstrating the effectiveness of our approach are given in §4. In §5, we give some concluding remarks.

2 2D Hermitian Dirac-Wilson formulation

Following [Reb03], we describe here the 2D Dirac-Wilson operator, H , and the attendant system of linear equations, $H(\mathbf{u})\mathbf{f} = \mathbf{b}$. The values of the gauge variables, \mathbf{u} , are given as $e^{i\theta}$ and, thus, are unitary, complex, and scalar valued. The distribution of the phase angles, θ , depends on the “temperature” of the physical system, prescribed by parameter β . For $\beta \rightarrow \infty$, corresponding to a cold temperature of the physical system, the distribution is *smooth* ($\lim_{\beta \rightarrow \infty} \mathbf{u} \equiv 1$). For realistic values of β , between 2 and 6, the system temperature is said to be hot, and the phases are randomly distributed.

The domain of interest is a 2D periodic $N \times N$ uniform lattice (grid), where the lattice sites (gridpoints) are distance $h = 1$ apart. Larger systems are thus obtained by enlarging N , and not by moving lattice points closer together. The fermionic degrees of freedom are defined at the gridpoints on the lattice, while the gauge variables are defined on the lattice edges, as shown in Figure 1. At every gridpoint, x , the unknown function is a vector of length 2:

$$\mathbf{f}(x) = \begin{pmatrix} \mathbf{f}(x, s = 1) \\ \mathbf{f}(x, s = 2) \end{pmatrix} = \begin{pmatrix} \mathbf{v}(x) \\ \mathbf{w}(x) \end{pmatrix},$$

where $s = 1, 2$ are spin indices, with spin corresponding to angular momentum.

Let \hat{m} be the unit vector in coordinate directions $m = 1, 2$ and $\mathbf{u}(x, m)$ be the gauge variable located at the link associated with gridpoints x and $x + \hat{m}$. Then the action of H is defined in terms of the covariant difference operators,

$$(\nabla_m^+ \mathbf{f})(x, s) = \mathbf{u}(x, m) \mathbf{f}(x + \hat{m}, s) - \mathbf{f}(x, s) \quad (1)$$

$$(\nabla_m^- \mathbf{f})(x, s) = \mathbf{f}(x, s) - \mathbf{u}(x - \hat{m}, m)^* \mathbf{f}(x - \hat{m}, s), \quad (2)$$

and the Pauli matrices,

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = -i\sigma_1\sigma_2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The action of the Pauli matrices are denoted by $\sigma_m \mathbf{f}$. Explicitly,

$$(\sigma_m \mathbf{f})(x, s) = \sum_{s'} (\sigma_m)_{s, s'} \mathbf{f}(x, s').$$

With these definitions, H is defined implicitly by its action on $\mathbf{f}(x, s)$ at lattice site x :

$$\begin{aligned} (H\mathbf{f})(x, s) = \sigma_3 \left[\sum_{m=1}^2 \frac{1}{2h} \sigma_m (\nabla_m^+ + \nabla_m^-) \mathbf{f}(x, s) \right. \\ \left. + \frac{1}{2h} \sum_{m=1}^2 (-\nabla_m^+ + \nabla_m^-) \mathbf{f}(x, s) + \rho \mathbf{f}(x, s) \right], \end{aligned} \quad (3)$$

where ρ is the relative quark mass and $h = 1$; h is included here to emphasize the comparison to familiar matrices from PDEs, and is used later in §3 to scale the matrix. Note that, due to the σ_3 term in (3), H is Hermitian and indefinite.

The corresponding system of linear equations can be written in the following two-by-two block form:

$$\begin{pmatrix} -\rho I - A & B \\ B^* & \rho I + A \end{pmatrix} \begin{pmatrix} \mathbf{v} \\ \mathbf{w} \end{pmatrix} = \begin{pmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \end{pmatrix}.$$

Operators $A, B \in \mathbb{C}^{n \times n}$, $n = N \times N$, are defined by their actions on the components of \mathbf{f} , corresponding to spin indices $s = 1, 2$. For example, using the local numbering in Figure 1, the actions of A and B on \mathbf{v} are given as follows:

$$(A\mathbf{v})_0 = \frac{1}{2h} (\bar{\mathbf{u}}_- \mathbf{v}_- + \mathbf{u}_+ \mathbf{v}_+ + \bar{\mathbf{u}}^- \mathbf{v}^- + \mathbf{u}^+ \mathbf{v}^+) - \frac{2}{h} \mathbf{v}_0, \quad (4)$$

$$(B\mathbf{v})_0 = \frac{1}{2h} (\mathbf{u}_+ \mathbf{v}_+ - \bar{\mathbf{u}}_- \mathbf{v}_- - i\mathbf{u}^+ \mathbf{v}^+ + i\bar{\mathbf{u}}^- \mathbf{v}^-). \quad (5)$$

The right side, \mathbf{b} , is called the *fermionic source vector* and is equal to one at a given gridpoint x and is zero elsewhere.

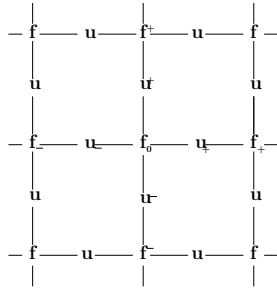


Fig. 1. Local numbering of the unknowns, \mathbf{f} , and gauge field coefficients, \mathbf{u} , used in the definition of the operators A and B .

3 Spectral properties of the Dirac system

In this section, we analyze the properties of the 2D Hermitian Dirac-Wilson operator, H , for different values of the relative quark mass, ρ , and temperature parameter, β . In particular, we consider the dependence of the conditioning of H on ρ , recalling that, as ρ approaches its physical value, H becomes nearly singular.

We begin with an analysis of H in the absence of an external field (i.e., $\mathbf{u} \equiv 1$), referred to as the “free” case. For $\mathbf{u} \equiv 1$, the covariant difference operators defined in (1) and (2) reduce to the standard first-order forward and backward difference operators. It is easy to see that, for $\mathbf{u} \equiv 1$, A and B in (4) and (5) have zero-row-sum. Hence, H is singular for $\rho = 0$, and H becomes nearly singular for $0 < \rho \ll 1$, the physical value of ρ for $\mathbf{u} \equiv 1$.

Recall that H is indefinite. Considering a (preconditioned) conjugate gradient algorithm, the equivalent system of normal equations,

$$H^* H \mathbf{f} = H^* \mathbf{b}, \quad (6)$$

can be solved instead. Given an eigenpair, (λ, \mathbf{x}) , of H , we have $H^* H \mathbf{x} = \lambda^2 \mathbf{x}$, so the normal form also becomes increasingly ill-conditioned as $\rho \rightarrow 0$, since the maximum eigenvalue remains $O(1)$ for all ρ . Clearly, CG is inefficient as a stand-alone solver for this system. However, classical multigrid provides a suitable preconditioner in this “free” case, as can be easily seen by relating H^2 to a decoupled two-by-two system of partial differential equations (PDEs) as follows.

Consider the equivalent system, where the problem is rescaled such that $h = \frac{1}{N-1} \rightarrow 0$ on a fixed domain. For $\mathbf{u} \equiv 1$, $A = \frac{h}{2} \Delta_h$ and $B^* B = B B^* = -\Delta_h$, where Δ_h denotes the five-point discrete Laplacian obtained using second-order centered differences. Thus, $H^* H$ has the following two-by-two block diagonal form:

$$H^*H = \begin{pmatrix} -\rho I - A & B \\ B^* & \rho I + A \end{pmatrix}^2 = \begin{pmatrix} (\rho I + \frac{h}{2}\Delta_h)^2 - \Delta_h & 0 \\ 0 & (\rho I + \frac{h}{2}\Delta_h)^2 - \Delta_h \end{pmatrix}.$$

Denoting the diagonal blocks by C , for $\rho = 0$ we have $C = -\Delta_h(I - \frac{h^2}{4}\Delta_h)$. Since $\sigma(-\Delta_h) \subseteq [0, \frac{8}{h^2}]$, we have that $\sigma(I - \frac{h^2}{4}\Delta_h) \subseteq [1, 3]$, implying C is spectrally equivalent to $-\Delta_h$. The theory of equivalent preconditioning [FMP89] then suggests that preconditioning C with a standard multigrid method for the Laplacian would be efficient. We note that, in practice, if we apply an AMG-preconditioned CG, we observe good solver performance for physical values of the quark mass (i.e., $0 < \rho \ll 1$) as well.

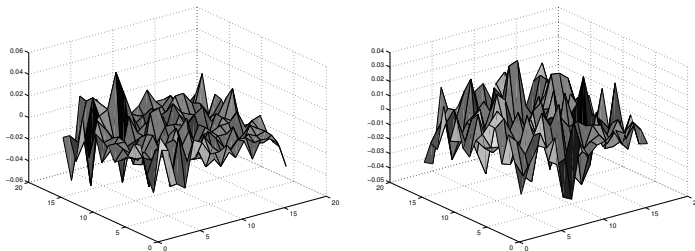


Fig. 2. Real (left) and complex (right) algebraically smooth error of H^2 for $m_q = .05, \beta = 3$ and $N = 16$. This error was computed using 200 Gauss-Seidel iterations on $H^2\mathbf{f} = \mathbf{0}$ with a random initial guess for \mathbf{f} .

We now focus on the more challenging case with the presence of the gauge field, when H^2 is no longer a block diagonal system. Unfortunately, in the presence of an external field, where \mathbf{u} is random (e.g., $\beta \in [2, 6]$), H^2 does not appear to be related to any standard system of PDEs. However, similar to the free case, H is indefinite and H^2 becomes ill conditioned as ρ approaches its critical value. More precisely, take $\rho = 0$ for H defined in (3) and let $\hat{H} = \sigma_3 H$. \hat{H} is then non-Hermitian and has eigenvalues with positive *real part*. The critical value of the quark mass, ρ_{cr} , is then defined by $\rho_{cr} = \min_i |\Re(\lambda_i(\hat{H}))|$. For physical values of ρ , the *mass gap*, $m_q := \rho - \rho_{cr}$, tends to zero, and H^2 becomes near-singular. This is the primary reason that all existing local algorithms grow in computational complexity for the Dirac system as the relative quark mass approaches its physical value, a phenomenon referred to as *critical slowing down*.

An additional difficulty, not encountered in the free case, is that the near-kernel components of H and, hence, H^*H , are locally oscillatory. This is demonstrated in Figure 2, where plots of the real and imaginary parts of a near-kernel component, computed using 200 iterations of Gauss-Seidel on the homogeneous problem, are given. Our experiments indicate that this oscillatory local character of the near-kernel components is dependent on the distribution of the gauge field, which is itself randomly specified.

To successfully solve the Dirac system for the random case, it is imperative that our iterative solver be able to efficiently attenuate such error components. Standard geometric and algebraic multigrid methods typically construct coarse-level corrections based on the assumption that the error not effectively reduced by the multigrid relaxation procedure is locally constant or, in general, smooth in the geometric sense, and would thus not be immediately suitable as a solver for this random case.

Smoothed aggregation multigrid (SA) [VMB96] was designed to allow efficient attenuation of error in a subspace characterized locally by a given set of error components, regardless of whether these are smooth or oscillatory in nature. The Dirac system poses an additional difficulty for the iterative solver, in that an a priori knowledge of these near-kernel components is not available. For this reason, we use the recently developed adaptive version of the smoothed aggregation multigrid method (α SA, [BFM⁺04]), which allows its setup procedure to identify the requisite error components and modify the method to ensure they can be efficiently eliminated. The α SA setup procedure is a multilevel scheme based on the power method for the error propagation operator of the method itself. In the interest of brevity, we refer for details of the method to [BFM⁺04].

4 Numerical results

This present section reports on numerical results obtained by applying various solvers to the 2D Dirac system defined in §2. We solve the equivalent normal system of equations, (6), reformulated as a two-by-two block *real* system,

$$\begin{bmatrix} X & -Y \\ Y & X \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} = \begin{bmatrix} \mathbf{c}_1 \\ \mathbf{c}_2 \end{bmatrix}, \quad (7)$$

where X, Y are real-valued matrices that satisfy $H^*H = X + iY$, $\mathbf{f} = \mathbf{x} + i\mathbf{y}$, and $H^*\mathbf{b} = \mathbf{c}_1 + i\mathbf{c}_2$.

Results of our numerical experiments are given in Table 1. The experiments were carried out on the problem with $\mathbf{b} = \mathbf{0}$ and random initial guesses for $[\mathbf{x}, \mathbf{y}]^T$. For the α SA preconditioner, we used 3 level $V(2,2)$ -cycles with an SOR-type relaxation. We note that, due to the more aggressive coarsening used in smoothed aggregation multigrid, $V(2,2)$ cycles are commonly used even when solving the Poisson equation. For the reported results, eight near-kernel components were computed in the adaptive setup and used to define the transfer operators of the α SA preconditioner. In the α SA preconditioned conjugate gradient (CG) results, one iteration of the resulting SA cycle was used as a preconditioner in the CG iteration. The Krylov solver used for comparison in Table 1 was a standard diagonally preconditioned CG iteration.

In current state-of-the-art QCD simulations, typical problem sizes are $N = 32$ and 64 . As already mentioned, the asymptotic convergence factors

	.01	.05	.1	.3		.01	.05	.1	.3
2	.25 / .98	.27 / .96	.24 / .91	.22 / .83	2	.33 / .99	.31 / .96	.31 / .94	.31 / .85
3	.29 / .98	.27 / .94	.26 / .92	.27 / .84	3	.42 / .98	.42 / .97	.40 / .93	.31 / .86
5	.28 / .96	.29 / .95	.26 / .92	.25 / .81	5	.31 / .99	.31 / .96	.29 / .92	.28 / .83

Table 1. Average convergence factors for α SA preconditioned CG and diagonally preconditioned CG applied to (7) with $N = 32$ (left) and $N = 64$ (right), for various choices of the mass gap, m_q , and several values of the temperature parameter, β .

of existing solvers applied to the Dirac system quickly tend towards one for critical choices of mass and temperature. This is demonstrated in Table 1 for diagonally preconditioned CG. Further, the numerical results in Table 1 suggest that when using eight computed near-kernel components in defining the SA interpolation operators, the asymptotic convergence factor of α SA preconditioned CG remains uniformly bounded away from one for $\beta \in [2.0, 6.0]$ and $\rho \rightarrow \rho_{cr}$. This is the main result of this paper, and the first such result to date.

To obtain a more complete picture of the overall effectiveness of our multi-grid iteration, we examine also *operator complexity*, defined as the number of nonzero entries stored in the operators on all levels divided by the number of nonzero entries in the finest-level matrix. The operator complexity can be viewed as indicating how expensive the entire V -cycle is compared to performing only the finest-level relaxations of the V -cycle. Even though we use eight near-kernel components to define prolongation, the operator complexity in our experiments stayed bounded by 3.0. These low values result from the fact that the problem size is aggressively reduced in forming the smoothed aggregation coarse problems.

One drawback of using the adaptive version of SA is the nontrivial cost associated with identifying the error components on which we base the transfer operators in SA. Of course, the hope is that this cost is optimal in that it is proportional to the number of degrees of freedom in the problem. Our experiments suggest that this is so. Further, a QCD simulation requires solving the system of equations for many right sides, whereas the adaptive SA setup is performed only once, with the resulting method used to solve the system with many right sides. For the results reported here, even with the cost of the adaptive setup, the resulting SA method is more efficient than a diagonally preconditioned CG algorithm when solving with a small number ($O(1)$) of right sides. Indeed, for the experiments considered in Table 1, only four right sides need be solved to justify the cost of the adaptive setup for the smallest value of mass gap ($m_q = .01$), i.e., the most ill conditioned system. For example, with $\beta = 3$ and $m_q = .01$, the CPU time required for the adaptive setup was 13.7 seconds and the CPU time needed to reduce the relative residual by a factor of 10^5 for a single right side, using α SA preconditioned CG, was 0.8 seconds. Solving the same system using diagonally preconditioned CG required 4.7 sec CPU time.

5 Conclusions

Our experiments demonstrate that α SA provides an efficient preconditioner for the 2D lattice QCD problems considered. We note that the cost of each iteration critically depends on the ratio of the number of degrees of freedom on the fine level to that on the coarser level. The coarsening for our 2D problem was very aggressive, leading to acceptable operator complexities even with eight adaptively computed near-kernel components. It remains to be verified whether these favorable 2D results carry over to the full 4D case.

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