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# An object oriented code for simulating supersymmetric Yang–Mills theories

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#### Abstract

Discretization of supersymmetric Yang–Mills (SYM) theories is an old problem in lattice field theory. It has resisted solution until recently when new ideas drawn from orbifold constructions and topological field theories have been brought to bear on the question. The result has been the creation of a new class of lattice gauge theories in which the lattice action is invariant under one or more supersymmetries. The resultant theories are local, free of doublers and also possess exact gauge-invariance. In principle they form the basis for a truly non-perturbative definition of the continuum SYM theories. In the continuum limit they lead to a version of the Yang-Mills theory formulated in terms of *twisted* fields. In this paper, we briefly review these ideas and then go on to describe the details of a C++ code, which can be used to simulate these theories. We sketch the design of the code, with particular emphasis being placed on SYM theories with  $\mathcal{N} = 2$  in two dimensions and  $\mathcal{N} = 4$  in three and four dimensions, making one-to-one comparisons between the essential components of the SYM theories and their corresponding counterparts appearing in the simulation code.

*Keywords:* Lattice Gauge Theory, Supersymmetric Yang–Mills, Rational Hybrid Monte Carlo, Object Oriented Programming

#### 1. Introduction

The problem of formulating supersymmetric theories on lattices has a long history going back to the earliest days of lattice gauge theory. However, after initial efforts failed to produce useful supersymmetric lattice actions the topic languished for many years. Indeed a folklore developed that supersymmetry

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and the lattice were mutually incompatible. However, recently, the problem has been re-examined using new tools and ideas such as topological twisting [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15], orbifold projection and deconstruction [16, 17, 18, 19, 20, 21, 22, 23, 24, 25], and a class of lattice models have been constructed which maintain one or more supersymmetries exactly at non-zero lattice spacing<sup>2</sup>.

The availability of a supersymmetric lattice construction is clearly very exciting. For example, having a lattice construction of the well known  $\mathcal{N} = 4$  SYM in four-dimensions is very advantageous from the point of view of exploring the connection between gauge theories and string/gravitational theories. But even without this connection to string theory, it is clearly of great importance to be able to give a non-perturbative formulation of a supersymmetric theory via a lattice path integral, in the same way that one can formally define QCD as a limit of lattice QCD as the lattice spacing goes to zero and the box size to infinity. From a practical point of view, one can also hope that some of the technology of lattice field theory such as strong coupling expansions and Monte Carlo simulation can be brought to bear on such supersymmetric theories.

In this paper, we will briefly describe the key ingredients that go into the lattice constructions of a variety of SYM theories and then provide the details of C++ code that can be used to simulate these theories. We hope that this work will motivate elementary particle physicists as well as high energy computational physicists to pursue numerical studies of supersymmetric lattice theories in particular, the  $\mathcal{N} = 4$  Yang-Mills in four dimensions.

#### 2. The method of topological twisting in SYM theories

First, let us explain why discretization of supersymmetric theories resisted solution for so long. The central problem is that naive discretizations of continuum supersymmetric theories break supersymmetry completely and radiative effects lead to a profusion of relevant supersymmetry breaking counterterms in the renormalized lattice action. The coefficients to these counterterms must then be carefully fine tuned as the lattice spacing is sent to zero in order to arrive at a supersymmetric theory in the continuum limit. In most cases this is both unnatural and practically impossible – particularly if the theory contains scalar fields. Of course, one might have expected problems – the supersymmetry algebra is an extension of the Poincaré algebra, which is explicitly broken on the lattice. Specifically, there are no infinitesimal translation generators on a discrete spacetime so that the algebra  $\{Q, \overline{Q}\} = \gamma_a p_a$ , where a is the spacetime index, is already broken at the classical level. Equivalently, it is a straightforward exercise to show that a naive supersymmetry variation of a naively discretized supersymmetric theory fails to yield zero as a consequence of the failure of the Leibniz rule when applied to lattice difference operators. In the

 $<sup>^{2}</sup>$ There exist other attempts to study various supersymmetric models on the lattice. See [26, 27, 28, 29, 30, 31, 32, 33].

last five years or so this problem has been revisited using new theoretical tools and ideas and a set of lattice models have been constructed which retain exactly some of the continuum supersymmetry at non-zero lattice spacing. The basic idea is to maintain a particular subalgebra of the full supersymmetry algebra in the lattice theory. The hope is that this exact symmetry will constrain the effective lattice action and protect the theory from dangerous supersymmetry violating counterterms.

Two approaches have been pursued to produce such supersymmetric actions: one based on ideas drawn from the field of topological field theory [1, 4, 5] and another pioneered by David B. Kaplan. Mithat Ünsal and collaborators using ideas of orbifolding and deconstruction [18, 19, 20]. Remarkably, these two seemingly independent approaches lead to the same lattice theories – see [12, 21, 22, 34] and the recent reviews [15, 35]. This convergence of two seemingly completely different approaches to the problem leads one to suspect that the final lattice theories may represent essentially unique solutions to the simultaneous requirements of locality, gauge-invariance and at least one exact supersymmetry. In this paper, we will use the language of topological twisting to discuss these supersymmetric lattice constructions, but the reader should remember that the orbifold methods lead to the same lattice theories.

#### 2.1. Twisting the supersymmetries in d dimensions

The basic idea of twisting goes back to Witten in his seminal paper on topological field theory [36] but actually had been anticipated in earlier work on staggered fermions [37]. In our context the idea is decompose the fields of the theory in terms of representations not of the original (Euclidean) rotational symmetry  $SO_{rot}(d)$  but a twisted rotational symmetry SO(d)', which is the diagonal subgroup of this symmetry and an  $SO_{\rm R}(d)$  subgroup of the R-symmetry of the theory,

$$SO(d)' = \operatorname{diag}(SO_{\operatorname{Lorentz}}(d) \times SO_{\operatorname{R}}(d))$$
 . (1)

To be explicit, consider the case where the total number of supersymmetries is  $Q = 2^d$ . In this case we can treat the supercharges of the twisted theory as a  $2^{d/2} \times 2^{d/2}$  matrix q. This matrix can be expanded on products of gamma matrices:

$$q = \mathcal{Q}I + \mathcal{Q}_a \gamma_a + \mathcal{Q}_{ab} \gamma_a \gamma_b + \dots$$
<sup>(2)</sup>

The  $2^d$  antisymmetric tensor components that arise in this basis are the twisted supercharges and satisfy a corresponding supersymmetry algebra following from the original algebra

$$\mathcal{Q}^2 = 0 , \qquad (3)$$

$$\{\mathcal{Q}, \mathcal{Q}_a\} = p_a , \qquad (4)$$

The presence of the nilpotent scalar supercharge Q is most important: it is the algebra of this charge that we can hope to translate to the lattice. The second

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piece of the algebra expresses the fact that the momentum is the Q-variation of something, which makes plausible the statement that the energy-momentum tensor and hence the entire action can be written in Q-exact form<sup>3</sup>. Notice that an action written in such a Q-exact form is trivially invariant under the scalar supersymmetry, provided the latter remains nilpotent under discretization.

The rewriting of the supercharges in terms of twisted variables can be repeated for the fermions of the theory and yields a set of antisymmetric tensors  $(\eta, \psi_a, \chi_{ab}, \ldots)$ , which for the case of  $Q = 2^d$  matches the number of components of a real Kähler-Dirac field. This repackaging of the fermions of the theory into a Kähler-Dirac field is at the heart of how the discrete theory avoids fermion doubling as was shown by Becher, Joos and Rabin in the early days of lattice gauge theory [38, 39].

It is important to recognize that the transformation to twisted variables corresponds to a simple change of variables in flat space – one more suitable to discretization. A true topological field theory only results when the scalar charge is treated as a true BRST charge and attention is restricted to states annihilated by this charge. In the language of the supersymmetric parent theory such a restriction corresponds to a projection to the vacua of the theory. It is *not* employed in the lattice constructions we discuss in this paper.

#### 2.2. A warm up example: Twisted $\mathcal{N} = 2$ SYM in two dimensions

We look at the twisted  $\mathcal{N} = 2$  SYM in two dimensions as a warm up example. This theory satisfies our requirements for supersymmetric latticization: its R-symmetry possesses an SO(2) subgroup corresponding to rotations of the two degenerate Majorana fermions into each other. Explicitly the theory can be written in twisted form as

$$S = \frac{1}{g^2} \mathcal{Q} \int \operatorname{Tr} \left( \chi_{ab} \mathcal{F}_{ab} + \eta [\overline{\mathcal{D}}_a, \mathcal{D}_a] - \frac{1}{2} \eta d \right) . \tag{6}$$

The degrees of freedom are just the twisted fermions  $(\eta, \psi_a, \chi_{ab})$  previously described and a complex gauge field  $\mathcal{A}_a$ . The latter is built from the usual gauge field and the two scalars present in the untwisted theory  $\mathcal{A}_a = A_a + iB_a$  with corresponding complexified field strength  $\mathcal{F}_{ab}$ .

The complex covariant derivatives appearing in these expressions are defined by

$$\mathcal{D}_a = \partial_a + \mathcal{A}_a = \partial_a + A_a + iB_a , \overline{\mathcal{D}}_a = \partial_a + \overline{\mathcal{A}}_a = \partial_a + A_a - iB_a .$$
 (7)

All fields take values in the adjoint representation of  $U(N)^4$ . It should be noted that despite the appearance of a complexified connection and field strength the

 $<sup>^3</sup>Actually in the case of the four-dimensional <math display="inline">\mathcal{N}=4$  there is an additional  $\mathcal{Q}\text{-}closed$  term needed.

<sup>&</sup>lt;sup>4</sup>The generators are taken to be *anti-hermitian* matrices satisfying  $Tr(T^aT^b) = -\delta^{ab}$ .

theory possesses only the usual U(N) gauge-invariance corresponding to the real part of the gauge field.

Notice that the original scalar fields transform as vectors under the original R-symmetry and hence become vectors under the twisted rotation group while the gauge fields are singlets under the R-symmetry and so remain vectors under twisted rotations. This structure makes possible the appearance of a complex gauge field in the twisted theory.

The nilpotent transformations associated with  $\mathcal{Q}$  are given explicitly by

$$Q \mathcal{A}_{a} = \psi_{a}$$

$$Q \psi_{a} = 0$$

$$Q \overline{\mathcal{A}}_{a} = 0$$

$$Q \chi_{ab} = -\overline{\mathcal{F}}_{ab}$$

$$Q \eta = d$$

$$Q d = 0$$
(8)

Performing the Q-variation and integrating out the auxiliary field d yields

$$S = \frac{1}{g^2} \int \operatorname{Tr} \left( -\overline{\mathcal{F}}_{ab} \mathcal{F}_{ab} + \frac{1}{2} [\overline{\mathcal{D}}_a, \mathcal{D}_a]^2 - \chi_{ab} \mathcal{D}_{[a} \psi_{b]} - \eta \overline{\mathcal{D}}_a \psi_a \right) .$$
(9)

To untwist the theory and verify that indeed in flat space it just corresponds to the usual theory one can do a further integration by parts to produce

$$S = \frac{1}{g^2} \int \text{Tr} \left( -F_{ab}^2 + 2B_a D_b D_b B_a - [B_a, B_b]^2 + L_F \right) , \qquad (10)$$

where  $F_{ab}$  is the usual Yang–Mills term. It is now clear that the imaginary parts of the gauge fields  $B_a$  can now be given an interpretation as the scalar fields of the usual formulation. Similarly one can build spinors out of the twisted fermions and write the action in the manifestly Dirac form

$$L_F = \begin{pmatrix} \chi_{12} & \frac{\eta}{2} \end{pmatrix} \begin{pmatrix} -D_2 - iB_2 & D_1 + iB_1 \\ D_1 - iB_1 & D_2 - iB_2 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} .$$
(11)

2.3. Discretization of the twisted  $\mathcal{N} = 2$ , d = 2 theory

The twisted theory described in the previous section may be discretized using the techniques developed in [12, 22, 25]. (Complex) gauge fields are represented as complexified Wilson gauge links  $\mathcal{U}_a(\mathbf{n}) = e^{\mathcal{A}_a(\mathbf{n})}$  living on links  $(\mathbf{n}, \mathbf{n} + \hat{\boldsymbol{\mu}}_a)$  of a lattice, which for the moment we can think of as hypercubic. These transform in the usual way under U(N) lattice gauge transformations

$$\mathcal{U}_a(\mathbf{n}) \to G(\mathbf{n})\mathcal{U}_a(\mathbf{n})G^{\dagger}(\mathbf{n}+\widehat{\boldsymbol{\mu}}_a)$$
 (12)

Supersymmetric invariance then implies that  $\psi_a(\mathbf{n})$  live on the same links as  $\mathcal{U}_a(\mathbf{n})$  and transform identically. The scalar fermion  $\eta(\mathbf{n})$  is clearly most naturally associated with a site and transforms accordingly

$$\eta(\mathbf{n}) \to G(\mathbf{n})\eta(\mathbf{n})G^{\dagger}(\mathbf{n})$$
 (13)



Figure 1: The unit cell of the two-dimensional  $\mathcal{N}=2$  lattice SYM with the orientation assignments for twisted fields.

The field  $\chi_{ab}(\mathbf{n})$  is slightly more difficult. Naturally as a 2-form it should be associated with a plaquette. In practice we introduce diagonal links running through the center of the plaquette and choose  $\chi_{ab}(\mathbf{n})$  to lie with opposite orientation along those diagonal links. This choice of orientation will be necessary to ensure gauge-invariance. Figure 1 shows the unit cell of the resultant lattice theory.

To complete the discretization we need to describe how continuum derivatives are to be replaced by difference operators. A natural technology for accomplishing this in the case of adjoint fields was developed many years ago and yields expressions for the derivative operator applied to arbitrary lattice p-forms [40]. In the case discussed here we need just two derivatives given by the expressions

$$\mathcal{D}_{a}^{(+)}f_{b}(\mathbf{n}) = \mathcal{U}_{a}(\mathbf{n})f_{b}(\mathbf{n}+\widehat{\boldsymbol{\mu}}_{a}) - f_{b}(\mathbf{n})\mathcal{U}_{a}(\mathbf{n}+\widehat{\boldsymbol{\mu}}_{b}) , \qquad (14)$$

$$\overline{\mathcal{D}}_{a}^{(-)}f_{a}(\mathbf{n}) = f_{a}(\mathbf{n})\overline{\mathcal{U}}_{a}(\mathbf{n}) - \overline{\mathcal{U}}_{a}(\mathbf{n}-\widehat{\boldsymbol{\mu}}_{a})f_{a}(\mathbf{n}-\widehat{\boldsymbol{\mu}}_{a}) .$$
(15)

The lattice field strength is then given by the gauged forward difference  $\mathcal{F}_{ab}(\mathbf{n}) = \mathcal{D}_a^{(+)} \mathcal{U}_b(\mathbf{n})$  and is automatically antisymmetric in its indices. Furthermore, it transforms like a lattice 2-form and yields a gauge-invariant loop on the lattice when contracted with  $\chi_{ab}(\mathbf{n})$ . Similarly the covariant backward difference appearing in  $\overline{\mathcal{D}}_a^{(-)} \mathcal{U}_a(\mathbf{n})$  transforms as a 0-form or site field and hence can be contracted with the site field  $\eta(\mathbf{n})$  to yield a gauge-invariant expression.

This use of forward and backward difference operators guarantees that the solutions of the theory map one-to-one with the solutions of the continuum theory and hence fermion doubling problems are evaded [38]. Indeed, by introducing a lattice with half the lattice spacing one can map this Kähler-Dirac fermion action into the action for staggered fermions [41]. Notice that, unlike the case of QCD, there is no rooting problem in this supersymmetric construction since the additional fermion degeneracy is already required by the continuum theory. The number of fermions of the twisted theory exactly fills out the components

of a Kähler-Dirac field and corresponds to the taste degeneracy of (reduced) staggered fermions.

# 2.4. Twisted $\mathcal{N} = 4$ SYM in three dimensions

The twist of  $\mathcal{N} = 4$  SYM in three dimensions<sup>5</sup> can be most succinctly written in the form where

$$S = \frac{1}{g^2} Q \int d^3x \left( \chi_{ab} \mathcal{F}_{ab} + \eta \left[ \overline{\mathcal{D}}_a, \mathcal{D}_a \right] + \frac{1}{2} \eta d + B_{abc} \overline{\mathcal{D}}_c \chi_{ab} \right) .$$
(16)

The fermions comprise a multiplet of p-form fields  $(\eta, \psi_a, \chi_{ab}, \theta_{abc})^6$  where in three dimensions p = 0...3. This multiplet of twisted fermions corresponds to a single Kähler-Dirac field and here possesses eight single component fields as expected for a theory with  $\mathcal{N} = 4$  supersymmetry in three dimensions.

The imaginary parts of the complex gauge field  $\mathcal{A}_a \ a = 1...3$  appearing in this construction yield the three scalar fields of the conventional (untwisted) theory. Fields d and  $B_{abc}$  are auxiliaries introduced to render the scalar nilpotent supersymmetry Q nilpotent off shell. The latter acts on the twisted fields as follows

$$QA_{a} = \psi_{a}$$

$$Q\overline{A}_{a} = 0$$

$$Q\psi_{a} = 0$$

$$Q\chi_{ab} = \overline{\mathcal{F}}_{ab}$$

$$Q\eta = d$$

$$Qd = 0$$

$$QB_{abc} = \theta_{abc}$$

$$Q\theta_{abc} = 0$$
(17)

Notice that this construction differs slightly from the one discussed in [43]. The fermion term involving a 3-form is here trivially rewritten as a Q-exact rather than Q-closed form.

Doing the Q-variation, integrating out the field d and using the Bianchi identity

$$\epsilon_{abc}\overline{\mathcal{D}}_c\overline{\mathcal{F}}_{ab} = 0 , \qquad (18)$$

yields

$$S = \frac{1}{g^2} \int d^3x \operatorname{Tr} \left( -\overline{\mathcal{F}}_{ab} \mathcal{F}_{ab} + \frac{1}{2} [\overline{\mathcal{D}}_a, \mathcal{D}_a]^2 - \chi_{ab} \mathcal{D}_{[a} \psi_{b]} - \psi_a \overline{\mathcal{D}}_a \eta - \theta_{abc} \overline{\mathcal{D}}_{[c} \chi_{ab]} \right).$$
(19)

<sup>&</sup>lt;sup>5</sup>This twist of  $\mathcal{N} = 4$ , d = 3 SYM is known as the Blau-Thompson twist [42].

<sup>&</sup>lt;sup>6</sup>It is common in the continuum literature to replace the 2- and 3-form fields in these expressions by their Hodge duals; a second vector  $\hat{\psi}_a$  and scalar  $\hat{\eta}$  see, for example [42].



Figure 2: The unit cell of the three-dimensional  $\mathcal{N} = 4$  lattice SYM with the orientation assignments for twisted fermionic fields.

The terms appearing in the bosonic part of the action can then be written in the following form exposing the  $B_a$  dependence explicitly

$$\overline{\mathcal{F}}_{ab}\mathcal{F}_{ab} = (F_{ab} - [B_a, B_b])(F_{ab} - [B_a, B_b]) + (D_{[a}B_{b]})(D_{[a}B_{b]}) ,$$

$$\frac{1}{2} \left[\overline{\mathcal{D}}_a, \mathcal{D}_a\right]^2 = -2 \left(D_a B_a\right)^2 , \qquad (20)$$

where  $F_{ab}$  and  $D_a$  denote the usual field strength and covariant derivative depending on the real part of the connection  $\mathcal{A}_a$ .

# 2.5. Discretization of the three-dimensional $\mathcal{N} = 4$ SYM theory

The transition to the lattice from the continuum theory is similar to the case of the two-dimensional  $\mathcal{N} = 2$  SYM theory. We replace the continuum complex gauge field  $\mathcal{A}_a(x)$  at every point by an appropriate complexified Wilson link  $\mathcal{U}_a(\mathbf{n}) = e^{\mathcal{A}_a(\mathbf{n})}, a = 1...3$ . These lattice fields are taken to be associated with unit length vectors in the coordinate directions  $\mathbf{a}$  in an three-dimensional hypercubic lattice. By supersymmetry the fermion fields  $\psi_a(\mathbf{n}), a = 1...3$  lie on the same oriented link as their bosonic superpartners running from  $\mathbf{n} \to \mathbf{n} + \hat{\mu}_a$ . In contrast the scalar fermion  $\eta(\mathbf{n})$  is associated with the site  $\mathbf{n}$  of the lattice and the tensor fermions  $\chi_{ab}(\mathbf{n}), a < b = 1...3$  with a set of diagonal face links running from  $\mathbf{n} + \hat{\mu}_a + \hat{\mu}_b \to \mathbf{n}$ . The final 3-form field  $\theta_{abc}(\mathbf{n})$  is then naturally placed on the body diagonal running from  $\mathbf{n} \to \mathbf{n} + \hat{\mu}_a + \hat{\mu}_b + \hat{\mu}_c$ . The unit cell and fermionic field orientations of the three-dimensional theory is given in figure 2. The construction then posits that all link fields transform as bi-fundamental fields under gauge transformations

$$\begin{aligned} \eta(\mathbf{n}) &\to G(\mathbf{n})\eta(\mathbf{n})G^{\dagger}(\mathbf{n}) \\ \psi_{m}(\mathbf{n}) &\to G(\mathbf{n})\psi_{m}(\mathbf{n})G^{\dagger}(\mathbf{n}+\widehat{\boldsymbol{\mu}}_{m}) \\ \chi_{mn}(\mathbf{n}) &\to G(\mathbf{n}+\widehat{\boldsymbol{\mu}}_{m}+\widehat{\boldsymbol{\mu}}_{n})\chi_{mn}(\mathbf{n})G^{\dagger}(\mathbf{n}) \\ \theta_{mnq}(\mathbf{n}) &\to G(\mathbf{n})\theta_{mnq}(\mathbf{n})G^{\dagger}(\mathbf{n}+\widehat{\boldsymbol{\mu}}_{m}+\widehat{\boldsymbol{\mu}}_{n}+\widehat{\boldsymbol{\mu}}_{q}) \\ \mathcal{U}_{m}(\mathbf{n}) &\to G(\mathbf{n})\mathcal{U}_{m}(\mathbf{n})G^{\dagger}(\mathbf{n}+\widehat{\boldsymbol{\mu}}_{m}) \\ \overline{\mathcal{U}}_{m}(\mathbf{n}) &\to G(\mathbf{n}+\widehat{\boldsymbol{\mu}}_{m})\overline{\mathcal{U}}_{m}(\mathbf{n})G^{\dagger}(\mathbf{n}) \end{aligned}$$
(21)

The action of the lattice theory resembles to its continuum cousin with the one modification that the continuum field  $\mathcal{A}_a(x)$  is replaced with the Wilson link  $\mathcal{U}_m(\mathbf{n})$  and the lattice field strength being defined as  $\mathcal{F}_{mn}(\mathbf{n}) = \mathcal{D}_m^{(+)} \mathcal{U}_n(\mathbf{n})$ . Thus the supersymmetric and gauge-invariant lattice action is

$$S = \mathcal{Q} \sum_{\mathbf{n},m,n,q} \operatorname{Tr} \left( \chi_{mn}(\mathbf{n}) \mathcal{F}_{mn}(\mathbf{n}) + \eta(\mathbf{n}) \overline{\mathcal{D}}_{m}^{(-)} \mathcal{U}_{m}(\mathbf{n}) \right. \\ \left. + \frac{1}{2} \eta(\mathbf{n}) d(\mathbf{n}) + B_{mnq}(\mathbf{n}) \overline{\mathcal{D}}_{q}^{(+)} \chi_{mn}(\mathbf{n}) \right)$$
(22)

The covariant difference operators appearing in these expressions are defined by [25]

$$\mathcal{D}_m^{(-)} f_m(\mathbf{n}) = \mathcal{U}_m(\mathbf{n}) f_m(\mathbf{n}) - f_m(\mathbf{n} - \widehat{\boldsymbol{\mu}}_m) \mathcal{U}_m(\mathbf{n} - \widehat{\boldsymbol{\mu}}_m)$$
(23)

$$\mathcal{D}_m^{(+)} f_n(\mathbf{n}) = \mathcal{U}_m(\mathbf{n}) f_n(\mathbf{n} + \widehat{\boldsymbol{\mu}}_m) - f_n(\mathbf{n}) \mathcal{U}_m(\mathbf{n} + \widehat{\boldsymbol{\mu}}_n)$$
(24)

$$\overline{\mathcal{D}}_{m}^{(-)}f_{m}(\mathbf{n}) = f_{m}(\mathbf{n})\overline{\mathcal{U}}_{m}(\mathbf{n}) - \overline{\mathcal{U}}_{m}(\mathbf{n} - \widehat{\boldsymbol{\mu}}_{m})f_{m}(\mathbf{n} - \widehat{\boldsymbol{\mu}}_{m})$$
(25)

$$\overline{\mathcal{D}}_{m}^{(+)}f_{nq}(\mathbf{n}) = f_{nq}(\mathbf{n}+\widehat{\boldsymbol{\mu}}_{m})\overline{\mathcal{U}}_{m}(\mathbf{n}) - \overline{\mathcal{U}}_{m}(\mathbf{n}+\widehat{\boldsymbol{\mu}}_{n}+\widehat{\boldsymbol{\mu}}_{q})f_{nq}(\mathbf{n})$$
(26)

These expressions are determined by the twin requirements that they reduce to the corresponding continuum results for the adjoint covariant derivative in the naive continuum limit  $\mathcal{U}_m \to \mathbb{I} + \mathcal{A}_m$  and that they transform under gauge transformations like the corresponding lattice link field carrying the same indices. This allows the terms in the action to correspond to gauge-invariant closed loops on the lattice.

Upon following the prescription [25] for lattice covariant derivatives, we write down the lattice action in terms of the link fields  $\mathcal{U}_m(\mathbf{n})$  and  $\overline{\mathcal{U}}_m(\mathbf{n})$ 

$$S = \frac{1}{g^2} \sum_{\mathbf{n},m,n,q} \operatorname{Tr} \left( -\overline{\mathcal{F}}_{mn}(\mathbf{n}) \mathcal{F}_{mn}(\mathbf{n}) + \frac{1}{2} \left( \overline{\mathcal{D}}_m^{(-)} \mathcal{U}_m(\mathbf{n}) \right)^2 - \chi_{mn}(\mathbf{n}) \mathcal{D}_{[m}^{(+)} \psi_{n]}(\mathbf{n}) - \eta(\mathbf{n}) \overline{\mathcal{D}}_m^{(-)} \psi_m(\mathbf{n}) - \theta_{mnq}(\mathbf{n}) \overline{\mathcal{D}}_{[q}^{(+)} \chi_{mn]}(\mathbf{n}) \right)$$
(27)

The bosonic part of the action is

$$S_{B} = \frac{1}{g^{2}} \sum_{\mathbf{n},m,n} \operatorname{Tr} \left[ -\left(\overline{\mathcal{D}_{m}^{(+)}}\mathcal{U}_{n}(\mathbf{n})\right) \left(\mathcal{D}_{m}^{(+)}\mathcal{U}_{n}(\mathbf{n})\right) + \frac{1}{2} \left(\overline{\mathcal{D}}_{m}^{(-)}\mathcal{U}_{m}(\mathbf{n})\right)^{2} \right]$$
  
$$= \frac{1}{g^{2}} \sum_{\mathbf{n},m,n} \operatorname{Tr} \left[ \left(\overline{\mathcal{U}}_{n}(\mathbf{n}+\widehat{\boldsymbol{\mu}}_{m})\overline{\mathcal{U}}_{m}(\mathbf{n}) - \overline{\mathcal{U}}_{m}(\mathbf{n}+\widehat{\boldsymbol{\mu}}_{n})\overline{\mathcal{U}}_{n}(\mathbf{n})\right) \right]$$
$$\times \left(\mathcal{U}_{m}(\mathbf{n})\mathcal{U}_{n}(\mathbf{n}+\widehat{\boldsymbol{\mu}}_{m}) - \mathcal{U}_{n}(\mathbf{n})\mathcal{U}_{m}(\mathbf{n}+\widehat{\boldsymbol{\mu}}_{n})\right)$$
$$+ \frac{1}{2} \left(\mathcal{U}_{m}(\mathbf{n})\overline{\mathcal{U}}_{m}(\mathbf{n}) - \overline{\mathcal{U}}_{m}(\mathbf{n}-\widehat{\boldsymbol{\mu}}_{m})\mathcal{U}_{m}(\mathbf{n}-\widehat{\boldsymbol{\mu}}_{m})\right)^{2} \right]$$
(28)

and the fermionic part

$$S_{F} = -\frac{1}{g^{2}} \sum_{\mathbf{n},m,n,q,r,e,f} \operatorname{Tr} \left\{ \frac{1}{2} (\delta_{mq} \delta_{nr} - \delta_{mr} \delta_{nq}) \right. \\ \times \left[ \chi_{mn}(\mathbf{n}) \left( \mathcal{U}_{q}(\mathbf{n}) \psi_{r}(\mathbf{n} + \widehat{\boldsymbol{\mu}}_{q}) - \psi_{r}(\mathbf{n}) \mathcal{U}_{q}(\mathbf{n} + \widehat{\boldsymbol{\mu}}_{r}) \right) \right] \\ \left. + \eta(\mathbf{n}) \left( \psi_{m}(\mathbf{n}) \overline{\mathcal{U}}_{m}(\mathbf{n}) - \overline{\mathcal{U}}_{m}(\mathbf{n} - \widehat{\boldsymbol{\mu}}_{m}) \psi_{m}(\mathbf{n} - \widehat{\boldsymbol{\mu}}_{m}) \right) \right. \\ \left. + \frac{1}{3} (\delta_{mr} \delta_{ne} \delta_{qf} + \delta_{qr} \delta_{me} \delta_{nf} + \delta_{nr} \delta_{qe} \delta_{mf}) \right. \\ \left. \times \theta_{ref}(\mathbf{n}) \left( \chi_{re}(\mathbf{n} + \widehat{\boldsymbol{\mu}}_{f}) \overline{\mathcal{U}}_{f}(\mathbf{n}) - \overline{\mathcal{U}}_{f}(\mathbf{n} + \widehat{\boldsymbol{\mu}}_{r} + \widehat{\boldsymbol{\mu}}_{e}) \chi_{re}(\mathbf{n}) \right) \right\} .$$
(29)

It is easy to see that each term in the lattice action forms a gauge-invariant loop on the lattice.

# 2.6. Twisted $\mathcal{N} = 4$ SYM in four dimensions

In four dimensions the constraint that the target theory possess 16 supercharges singles out a single theory for which this construction can be undertaken  $-\mathcal{N} = 4$  SYM.

The continuum twist of  $\mathcal{N} = 4$  that is the starting point of the twisted lattice construction was first written down by Marcus in 1995 [44] although it now plays an important role in the Geometric-Langlands program and is, hence, sometimes called the GL-twist [45]. This four-dimensional twisted theory is most compactly expressed as the dimensional reduction of a five-dimensional theory in which the ten (one gauge field and six scalars) bosonic fields are realized as the components of a complexified five-dimensional gauge field while the 16 twisted fermions naturally span one of the two Kähler-Dirac fields needed in five dimensions. Remarkably, the action of this theory contains a  $\mathcal{Q}$ -exact piece of precisely the same form as the two dimensional theory given in (6) provided one extends the field labels to run now from one to five. In addition, the Marcus twist requires a new  $\mathcal{Q}$ -closed term, which was not possible in the two-dimensional theory.

$$S_{\text{closed}} = -\frac{1}{8} \int \operatorname{Tr} \epsilon_{mnpqr} \chi_{qr} \overline{\mathcal{D}}_p \chi_{mn} .$$
(30)

The supersymmetric invariance of this term then relies on the Bianchi identity

$$\epsilon_{mnpqr} \overline{\mathcal{D}}_p \overline{\mathcal{F}}_{qr} = 0 .$$
 (31)

# 2.7. Discretization of the four-dimensional $\mathcal{N} = 4$ SYM theory

In two and three dimensions we were able to accommodate the bosonic fields of the theory in a natural way by assigning them to the links of a hypercubic lattice. For the Q = 16 theory this is not possible; the theory can be parametrized in terms of five complex gauge fields in the continuum. We are thus motivated to search for a four dimensional lattice with five basis vectors  $\hat{\mu}_a a = 1...5$ . One simple solution is to use a hypercubic lattice with an additional body diagonal

$$\widehat{\boldsymbol{\mu}}_{1} = (1,0,0,0) 
\widehat{\boldsymbol{\mu}}_{2} = (0,1,0,0) 
\widehat{\boldsymbol{\mu}}_{3} = (0,0,1,0) 
\widehat{\boldsymbol{\mu}}_{4} = (0,0,0,1) 
\widehat{\boldsymbol{\mu}}_{5} = (-1,-1,-1,-1)$$
(32)

The field  $\mathcal{U}_5$  is then placed on the body diagonal link. Actually, we will indeed utilize such a hypercubic lattice when building the C++ data structure needed to code the resulting theory. Notice that the basis vectors sum to zero, consistent with the use of such a linearly dependent basis.

However, it should also be clear that a more symmetrical choice is possible in which the five basis vectors are entirely equivalent and the lattice theory possesses a large point group symmetry  $S^5$  corresponding to permutations of the set of basis vectors. Such a discrete structure exists in four dimensions: it is called the  $A_4^*$  lattice. It is constructed from the set of five basis vectors  $\hat{e}_a$  pointing from the center of a four-dimensional equilateral simplex out to its vertices together with their inverses  $-\hat{e}_a$ . It is the four-dimensional analog of the two-dimensional triangular lattice. A specific basis for the  $A_4^*$  lattice is given in the form of five lattice vectors

$$\widehat{e}_1 = \left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{6}}, \frac{1}{\sqrt{12}}, \frac{1}{\sqrt{20}}\right)$$
(33)

$$\widehat{e}_2 = \left(-\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{6}}, \frac{1}{\sqrt{12}}, \frac{1}{\sqrt{20}}\right)$$
 (34)

$$\widehat{e}_3 = \left(0, -\frac{2}{\sqrt{6}}, \frac{1}{\sqrt{12}}, \frac{1}{\sqrt{20}}\right)$$
 (35)

$$\widehat{e}_4 = \left(0, 0, -\frac{3}{\sqrt{12}}, \frac{1}{\sqrt{20}}\right)$$
(36)

$$\widehat{\boldsymbol{e}}_{5} = \left(0, 0, 0, -\frac{4}{\sqrt{20}}\right)$$
(37)

The basis vectors satisfy the relations

$$\sum_{m=1}^{5} \widehat{e}_m = 0; \ \widehat{e}_m \cdot \widehat{e}_n = \left(\delta_{mn} - \frac{1}{5}\right); \ \sum_{m=1}^{5} (\widehat{e}_m)_\mu (\widehat{e}_m)_\nu = \delta_{\mu\nu}; \ \mu, \nu = 1, \cdots, 4.$$
(38)

Notice that  $S^5$  is a subgroup of the twisted rotation symmetry group SO(4)'. Furthermore, the lattice fields transform in reducible representations of this discrete group - for example, the vector  $\mathcal{U}_a$  decomposes into a four component vector  $\mathcal{U}_{\mu}$  and a scalar field  $\phi = \sum_a \mathcal{U}_a$  under  $S^5$  and hence also under SO(4)' in the continuum limit. Invariance of the lattice theory with respect to  $S^5$  then guarantees that the lattice theory will inherit full invariance under twisted rotations as the lattice spacing is sent to zero.

Complexified Wilson gauge link variables  $\mathcal{U}_a$  are then placed on these links together with their  $\mathcal{Q}$ -superpartners  $\psi_a$ . The ten twisted fermions  $\chi_{ab}$  are associated with additional diagonal links  $\hat{e}_a + \hat{e}_b$  with a > b while a single fermion  $\eta$  is placed at each lattice site.

We can connect the basis vectors of the hypercubic lattice and the  $A_4^*$  lattice through a set of linear transformations - see [21, 46]. The integer-valued hypercubic lattice site vector **n** can be related to the physical location in spacetime using the  $A_4^*$  basis vectors  $\hat{e}_a$ 

$$\boldsymbol{R} = a \sum_{\nu=1}^{4} (\mu_{\nu} \cdot \mathbf{n}) \widehat{\boldsymbol{e}}_{\nu} = a \sum_{\nu=1}^{4} n_{\nu} \widehat{\boldsymbol{e}}_{\nu} , \qquad (39)$$

where *a* is the lattice spacing. On using the fact that  $\sum_{m} \hat{e}_{m} = 0$ , we can show that a small lattice displacement of the form  $d\mathbf{n} = \hat{\mu}_{m}$  corresponds to a spacetime translation by  $(a\hat{e}_{m})$ :

$$d\mathbf{R} = a \sum_{\nu=1}^{4} (\mu_{\nu} \cdot d\mathbf{n}) \widehat{\mathbf{e}}_{\nu} = a \sum_{\nu=1}^{4} (\widehat{\boldsymbol{\mu}}_{\nu} \cdot \widehat{\boldsymbol{\mu}}_{m}) \widehat{\mathbf{e}}_{\nu} = a \widehat{\mathbf{e}}_{m} .$$
(40)

The lattice action corresponds to a discretization of the Marcus twist on this  $A_4^*$  lattice and can be represented as a set of traced closed bosonic and fermionic loops. It is invariant under the exact Q scalar supersymmetry, lattice gauge transformations and a global permutation (point group) symmetry  $S^5$ , and can be proven free of fermion doubling problems as discussed before. The Q-exact part of the lattice action is again given by (9) with the indices  $\mu, \nu$  now labeling the five basis vectors of  $A_4^*$  or equivalently its hypercubic cousin.

Finally, it is important to note that while the true lattice in spacetime is this rather complicated looking  $A_4^*$  structure, we can represent all of the lattice fields in our theory by giving only their coordinates on the abstract hypercubic lattice. Indeed, since the lattice action only depends on the structure of the hypercubic lattice we will not need the explicit coordinates of the  $A_4^*$  lattice to generate Monte Carlo configurations during the simulation. The explicit mapping of hypercubic coordinates to spacetime coordinates in the  $A_4^*$  lattice is only needed when, for example, we want to compute spatially dependent objects such as correlation functions of fields. In this case we should compute distances relative to the underlying  $A_4^*$  lattice *not* its hypercubic partner.

While the supersymmetric invariance of the Q-exact term is manifest in the lattice theory it is not immediately clear how to discretize the continuum Q-closed term. Remarkably, it is possible to discretize (30) in such a way that it is indeed exactly invariant under the twisted supersymmetry:

$$S_{\text{closed}} = -\frac{1}{8} \sum_{\mathbf{n},m,n,p,q,r} \operatorname{Tr} \epsilon_{mnpqr} \chi_{qr} (\mathbf{n} + \widehat{\boldsymbol{\mu}}_m + \widehat{\boldsymbol{\mu}}_n + \widehat{\boldsymbol{\mu}}_p) \overline{\mathcal{D}}_p^{(-)} \chi_{mn} (\mathbf{n} + \widehat{\boldsymbol{\mu}}_p) , \quad (41)$$

which can be seen to be supersymmetric since the lattice field strength satisfies an exact Bianchi identity [40]

$$\epsilon_{mnpqr} \overline{\mathcal{D}}_p^{(+)} \overline{\mathcal{F}}_{qr} = 0 .$$
(42)

#### 3. Simulating the SYM theories: Algorithms

Although the fields entering into these twisted descriptions appear somewhat different to the usual fields used in QCD the basic algorithms we use to simulate them are borrowed directly from lattice QCD; namely we integrate out the fermions to produce a Pfaffian which is in turn represented by the square root of a determinant<sup>7</sup> and can be simulated using the usual RHMC algorithm [47].

If we denote the set of twisted fermions by the field  $\Psi = (\eta, \psi_{\mu}, \chi_{\mu\nu})$  we first introduce a corresponding pseudo-fermion field  $\Phi$  with action

$$S_{\rm PF} = \Phi^{\dagger} (M^{\dagger} M)^{-\frac{1}{4}} \Phi , \qquad (43)$$

where  $M = M(\mathcal{U}, \mathcal{U}^{\dagger})$  is the antisymmetric twisted lattice fermion operator given, for example, in  $(27)^8$ .

Integrating over the fields  $\Phi$  will then yield (up to a possible phase) the Pfaffian of the operator  $M(\mathcal{U}, \mathcal{U}^{\dagger})$  as required. The fractional power is approximated by the partial fraction expansion

$$\frac{1}{(M^{\dagger}M)^{\frac{1}{4}}} = \alpha_0 + \sum_{i=1}^{P} \frac{\alpha_i}{M^{\dagger}M + \beta_i} , \qquad (44)$$

where the coefficients  $\{\alpha_i, \beta_i\}$  are evaluated offline using the Remez algorithm to minimize the error in some interval  $(\epsilon, A)$ . Typically we have used P = 15which yields a fractional error of 0.00001 for the interval 0.0000001  $\rightarrow$  1000.0, which conservatively covers the range we are interested in.

 $<sup>^{7}</sup>$  Of course this ignores a possible sign ambiguity. We return to this issue later when we discuss whether the phase quenched simulations we use suffer from a sign problem.

<sup>&</sup>lt;sup>8</sup>The antisymmetry is guaranteed if the fermion action is rewritten as the sum of the original terms plus their lattice transposes.

Following the standard procedure, we introduce momenta  $(p_{\mathcal{U}}, p_F)$  conjugate to the coordinates  $(\mathcal{U}, \Phi)$  and evolve the coupled system using a discrete time leapfrog algorithm according to the classical Hamiltonian

$$H = S_B + S_{\rm PF} + p_{\mathcal{U}}\bar{p}_{\mathcal{U}} + p_{\Phi}\bar{p}_{\Phi} \ . \tag{45}$$

Notice that the bosonic  $\operatorname{action}^9$ 

$$S_B = \sum_{\mathbf{x},m,n} \operatorname{Tr} \left[ -\left( \overline{\mathcal{D}_m^{(+)} \mathcal{U}_n(\mathbf{x})} \right) \left( \mathcal{D}_m^{(+)} \mathcal{U}_n(\mathbf{x}) \right) + \frac{1}{2} \left( \overline{\mathcal{D}}_m^{(-)} \mathcal{U}_m(\mathbf{x}) \right)^2 \right], \quad (46)$$

is real, positive semi-definite in all these theories.

One step of the discrete time update is given by

$$\delta p_{\mathcal{U}} = \frac{\delta t}{2} \bar{f}_{\mathcal{U}} \tag{47}$$

$$\delta p_{\Phi} = \frac{\delta t}{2} \bar{f}_{\Phi} \tag{48}$$

$$\delta \mathcal{U} = \left( e^{\delta t p_{\mathcal{U}}} - I \right) \mathcal{U} \tag{49}$$

$$\delta \Phi = \delta t p_{\Phi} \tag{50}$$

$$\delta p_{\mathcal{U}} = \frac{\delta \iota}{2} \bar{f}_{\mathcal{U}} \tag{51}$$

$$\delta p_{\Phi} = \frac{\delta t}{2} \bar{f}_{\Phi} \tag{52}$$

where the forces  $f_{\mathcal{U}}$  and  $f_{\Phi}$  are given by

$$f_{\mathcal{U}} = -\frac{\delta S}{\delta \mathcal{U}} \tag{53}$$

$$f_{\Phi} = -\frac{\delta S}{\delta \Phi} \tag{54}$$

and the bar denotes complex conjugation. Using the partial fraction expansion given in (44) the fermionic contributions to these forces take the form

$$f_{\mathcal{U}}^{fermionic} = \sum_{i=1}^{P} \alpha_i \left[ \bar{t}_i \frac{\delta M}{\delta \mathcal{U}} s_i + \overline{\left( \bar{t}_i \frac{\delta M}{\delta \overline{\mathcal{U}}} s_i \right)} \right]$$
(55)

$$f_{\Phi}^{fermionic} = -\alpha_0 \bar{\Phi} - \sum_{i=1}^P \alpha_i \bar{s}_i \tag{56}$$

(57)

where

$$(M^{\dagger}M + \beta_i)s_i = \Phi \tag{58}$$

$$t_i = M s_i \tag{59}$$

<sup>&</sup>lt;sup>9</sup>From now on we interchangeably use  $\mathbf{x}$  and  $\mathbf{n}$  to denote the lattice site.

The latter set of sparse linear equations is solved using a multi-mass conjugate gradient (MCG) solver [48], which allows for the simultaneous solution of all P systems in a single CG solve.

At the end of one such classical trajectory the final configuration is subjected to a standard Metropolis test based on the Hamiltonian H. The symplectic and reversible nature of the discrete time update is then sufficient to allow for detailed balance to be satisfied and hence expectation values are independent of  $\delta t$ . After each such trajectory the momenta are refreshed from the appropriate Gaussian distribution as determined by H, which renders the simulation ergodic.

The fermionic contribution to the forces are shown below

$$f_{\mathcal{U}_{m}}^{fermionic} = \frac{\partial S_{pf}}{\partial \mathcal{U}_{m}} = \sum_{i=1}^{P} \alpha_{i} F^{\dagger} \frac{-1}{(M^{\dagger}M + \beta_{i})^{2}} \frac{\partial}{\partial \mathcal{U}_{m}} (M^{\dagger}M) F$$

$$= -\sum_{i=1}^{P} \alpha_{i} \left(\frac{F}{(M^{\dagger}M + \beta_{i})}\right)^{\dagger} \frac{\partial}{\partial \mathcal{U}_{m}} (M^{\dagger}M) \left(\frac{F}{(M^{\dagger}M + \beta_{i})}\right)$$

$$= -\sum_{i=1}^{P} \alpha_{i} \left(\frac{F}{(M^{\dagger}M + \beta_{i})}\right)^{\dagger} \left(M^{\dagger} \frac{\partial M}{\partial \mathcal{U}_{m}} + \frac{\partial M^{\dagger}}{\partial \mathcal{U}_{m}}M\right) \left(\frac{F}{(M^{\dagger}M + \beta_{i})}\right)$$

$$= -\sum_{i=1}^{P} \alpha_{i} \left[ \left(M \frac{F}{(M^{\dagger}M + \beta_{i})}\right)^{\dagger} \frac{\partial M}{\partial \mathcal{U}_{m}} \left(\frac{F}{(M^{\dagger}M + \beta_{i})}\right)$$

$$+ \left(\frac{F}{(M^{\dagger}M + \beta_{i})}\right)^{\dagger} \frac{\partial M}{\partial \mathcal{U}_{m}} \left(M \frac{F}{(M^{\dagger}M + \beta_{i})}\right) \right]$$

$$= -\sum_{i=1}^{P} \alpha_{i} \left[ t_{i}^{\dagger} \frac{\partial M}{\partial \mathcal{U}_{m}} s_{i} + s_{i}^{\dagger} \frac{\partial M^{\dagger}}{\partial \mathcal{U}_{m}} t_{i} \right]. \tag{60}$$

$$f_{F}^{fermionic} = \frac{\partial S_{pf}}{\partial F}$$

$$= \alpha_{0} \frac{\partial}{\partial F} (F^{\dagger}F) + \sum_{i=1}^{P} \alpha_{i} \frac{\partial}{\partial F} \left( F^{\dagger} \left[ (M^{\dagger}M + \beta_{i})^{-1}F \right] \right)$$

$$= \alpha_{0}F^{\dagger} + \sum_{i=1}^{P} \alpha_{i}s_{i}^{\dagger} . \qquad (61)$$

# 4. Overall structure of the C++ code

Typically the bosons lie on the usual nearest neighbour links of a hypercubic lattice while the fermions occupy both these links and additional site, face and body diagonal links. In the case of  $\mathcal{N} = 4$  in four dimensions we have to augment the set of boson links with one additional gauge field associated with the body diagonal link of the hypercube. We introduce the Lattice\_Vector class to store the coordinates of the lattice sites and also the vector between



Figure 3: The organizational structure of the C++ code that generates and measures field configurations.

sites. Such lattice vectors can be added or subtracted by overloading the '+' or '-' operators. These operations also respect the lattice boundary conditions. Associated with this class is a general function loop\_over\_lattice(x sites) that implements a loop over all lattice sites indexed by their coordinate vector; thus a simple loop looks like

#### while(loop\_over\_lattice(x,sites))....

The bosonic and pseudo fermionic fields are stored in various objects which are indexed via their lattice site vector and whose type corresponds directly to the tensor structure of the associated continuum field so that one finds C++ classes labeled Site\_Field, Link\_Field, Plaq\_Field, Body\_Field etc. in the header file utilities.h. The full Kähler-Dirac field is contained in the class Twist\_Fermion while the Gauge\_Field class contains the complexified Wilson gauge link. All these objects are are in turn built from objects of type Umatrix corresponding to complex NCOLOR x NCOLOR matrices. Simple arithmetric operations which overload the usual arithmetic operations are defined for manipulating these objects.

Let us briefly describe how the code works. The general organizational structure of the code is given in figure 3. We begin with sym.cpp. It reads the input parameters such as number of sweeps (SWEEPS), number of thermalization steps (THERM), gap in measurements (GAP), the 't Hooft coupling (LAMBDA), etc., using functions contained in the file read\_param.cpp. It can also read in previously generated field configurations using read\_in.cpp.

The code sym.cpp performs three major tasks:

- 1. Generates new configurations using a rational hybrid monte carlo (RHMC) algorithm. This is accomplished by calling the function update(U,F) contained in update.cpp
- 2. Saves the current field configuration after some number of Monte Carlo sweeps. (using the functions in write\_out.cpp)
- 3. Measures the observables in the theory. This is done by function calls within measure.cpp

Let us focus on the task of updating field configurations first. After reading the initial parameters and field configurations update() is called. Here we refresh the momenta p\_U and p\_F (using a Gaussian distribution) and then go to kinetic\_energy.cpp to compute the kinetic energy:

```
Adj(p_U)*p_U + Cjg(p_F)*p_F.
```

Compare this with the first two terms in the classical Hamiltonian (45):

$$\overline{p}_{\mathcal{U}}p_{\mathcal{U}} + \overline{p}_{\Phi}p_{\Phi}$$

After computing kinetic energy the boson and pseudo-fermion actions (45) are computed with a call to the function action().

The computation of the bosonic action  $S_B$  is straightforward. In the code it is accomplished with the line

KAPPA\*[0.5\*Tr(DmuUmu\*DmuUmu) + 2.0\*Tr(Fmunu\*Adj(Fmunu))] .

Here KAPPA is the dimensionless lattice coupling. It is defined in read\_param.cpp and depends on the number of dimensions (D), size of the lattice (LX, LY, LZ, T) and number of colors (NCOLOR).

The code associated with spefcific terms in the bosonic action can easily be identified with its analytic expression. We have

 $\begin{array}{l} \texttt{DmuUmu}(\texttt{x}) \rightarrow \texttt{Umu}(\texttt{x}) * \texttt{Udagmu}(\texttt{x}) - \texttt{Udagmu}(\texttt{x}-\texttt{e\_mu}) * \texttt{Umu}(\texttt{x}-\texttt{e\_mu}) \\ \texttt{Fmunu}(\texttt{x}) \rightarrow \texttt{Umu}(\texttt{x}) * \texttt{Umu}(\texttt{x}+\texttt{e\_mu}) - \texttt{Umu}(\texttt{x}) * \texttt{Umu}(\texttt{x}+\texttt{e\_nu}) \end{array}$ 

The code used to compute the fermionic part of the action is given by

 $\label{eq:s_F} \texttt{S_F} = \texttt{ampdeg*(Cjg(F)*F)} + \sum_{n=0}^{\texttt{DEGREE}} \texttt{amp[n]*(Cjg(F)*sol[n])} \;,$ 

where **n** runs from 0 to DEGREE (which is equal to number of terms in the Remez approximation P), ampdeg corresponds to  $\alpha_0$ , F the twisted pseudo-fermion F, Cjg(F) is  $F^{\dagger}$ , amp[n] is  $\alpha_i$  and sol[n] corresponds to  $s_i \equiv (M^{\dagger}M + \beta_i)^{-1}F$ .

Again one should compare this code with the form of the pseudo-fermion action

$$S_{pf} = \alpha_0 F^{\dagger} F + \sum_{i=1}^{P} \alpha_i F^{\dagger} \Big[ (M^{\dagger} M + \beta_i)^{-1} F \Big]$$

We invoke a multimass conjugate gradient solver MCG\_solver() given in MCG\_solver.cpp to help compute the terms needed in the fermionic action. The MCG solver can return the solutions to  $(M^{\dagger}M + \beta_i)s_i = F$  for all shifts  $\beta_i$ .

Once the Hamiltonian is computed we evolve the fields along a classical trajectory. This is handled by the function evolve\_fields. The evolution of the fields and momenta is achieved through a leapfrog algorithm. In the first half step we have

 $\begin{array}{rcl} p\_Umu & \rightarrow & p\_Umu + 0.5*DT*f\_Umu \\ p\_F & \rightarrow & p\_F + 0.5*DT*f\_F \\ Umu & \rightarrow & Umu + exp(DT*p\_Umu) \\ F & \rightarrow & F + DT*p\_F \end{array}$ 

Immediately after computing the change in fields (Umu and F) and momenta (p\_Umu and p\_F), we update the forces by calling force(). The bosonic force contribution to f\_Umu is given by

The computation of the fermionic force f\_F requires first a call to the MCG solver  $MCG_solver()$ . We find

$$f_F = -ampdeg*Cjg(F) - \sum_{n=0}^{DEGREE} amp[n]*Cjg(sol[n])$$

Once we have this solution an additional contribution to the gauge force coming from the pseudo-fermions is gotten by a call to the function fermion\_forces(). Each fermionic term in the action yields a contribution. We provide a part of this code in figure 4.

In the second half step of the leapfrog algorithm the momenta  $p_U$  and  $p_F$  are again updated with the new forces. These final forces are then saved for the next iteration.

In practice, it is important to use a multi-time step integrator for this evolution [49]. In this case while the fermions are evolved with a time step of DT, the bosons are integrated with the time step DT/MSTEP. Provided the boson force is substantially larger than the fermionic contribution this can result in fewer costly fermion inversions for a fixed acceptance rate. In practice the parameter MSTEPS can be tuned to optimize the update - typically MSTEPS=10.

Finally, control returns to update() and the updated Hamiltonian H\_new is computed. A simple Metropolis test is used to accept or reject the field configuration at the end of the trajectory.

```
#include "fermion_forces.h"
 1
2
3
    void fermion_forces(const Gauge_Field &U, Gauge_Field &f_U,
4
            const Twist_Fermion &s, const Twist_Fermion &p)
5
6
      Lattice_Vector x, e_mu;
7
      int sites, mu, a, b;
8
      Umatrix tmp;
9
      Gauge_Field Udag;
10
      Udag=Adj(U);
11
      f_U=Gauge_Field();
12
      //contribution to f_U from psi_muDb_mu(U)eta term
13
14
        sites = 0;
        while(loop_over_lattice(x,sites))
15
16
        {
          for(mu=0;mu<NUMLINK;mu++)</pre>
17
18
           {e_mu=Lattice_Vector(mu);
          tmp=Umatrix();
19
            for(a=0;a<NUMGEN;a++)</pre>
20
21
            {
              for(b=0;b<NUMGEN;b++)</pre>
22
23
              {tmp=tmp+conjug(p.getS().get(x).get(a))*s.getL().get(x,mu).get(b)
              *Lambda[a]*Lambda[b]*Udag.get(x,mu)-conjug(p.getS().get(x+e\_mu).get(a))
24
25
              *BC(x,e\_mu)*s.getL().get(x,mu).get(b)*Lambda[b]*Lambda[a]*Udag.get(x,mu);}
26
27
            f_U.set(x,mu,f_U.get(x,mu)-0.5*Adj(tmp));
28
         3
29
        sites=0;
30
        while(loop_over_lattice(x,sites))
31
        {
32
          for(mu=0;mu<NUMLINK;mu++)</pre>
33
           {e_mu=Lattice_Vector(mu);
          tmp=Umatrix();
34
35
            for(a=0;a<NUMGEN;a++)</pre>
36
            {
37
              for(b=0;b<NUMGEN;b++)</pre>
              \{tmp=tmp+conjug(p.getL().get(x,mu).get(a))*s.getS().get(x+e_mu).get(b)\}
38
39
              *BC(x,e\_mu)*Lambda[a]*Lambda[b]*Udag.get(x,mu)-
40
              conjug(p.getL().get(x,mu).get(a))*s.getS().get(x).get(b)
              *Lambda[b]*Lambda[a]*Udag.get(x,mu);}
41
42
43
            f_U.set(x,mu,f_U.get(x,mu)-0.5*Adj(tmp));
        }
44
45
        sites=0;
46
        while(loop_over_lattice(x,sites))
47
        for(mu=0;mu<NUMLINK;mu++) \{f_U.set(x,mu,-1.0*Adj(f_U.get(x,mu)));\}\}
48
     return;
49
    }
```

Figure 4: A part of the C++ code to compute the fermion force contribution.

```
class Link_Field{
 1
 2
    private:
 3
            Afield links[SITES][NUMLINK];
 4
    public:
            Link_Field(void);
 5
            Link_Field(int);
 6
 7
            Afield get(const Lattice_Vector &, const int) const;
 8
            void set(const Lattice_Vector &, const int, const Afield &);
 9
            void print(void);
10
            };
11
    Link_Field Cjg(const Link_Field &);
12
    Link_Field operator +(const Link_Field &, const Link_Field &);
13
14
    Link_Field operator -(const Link_Field &, const Link_Field &);
    Link_Field operator *(const double, const Link_Field &);
15
    Link_Field operator *(const Complex &, const Link_Field &);
16
    Complex operator *(const Link_Field &, const Link_Field &);
17
```

Figure 5: The Link\_Field class with overloading of operators (from utilities.h).

#### 4.1. Site, Link and Plaquette type operators

The bosonic and fermionic fields, and the covariant difference operators living on the hypercubic lattice are associated with various geometric structures such as sites, links and plaquettes. They are implemented in the code using various C++ classes: Site\_Field, Link\_Field, Plaq\_Field, Body\_Field, etc. They are constructed such that they can take values in U(N) or SU(N). They make appearances in the code in many ways and we summarize their general structure in the table below:

Site_Field	$S(\mathbf{x})$	$\overline{\mathcal{D}}_{\mu}^{(-)}L_{\mu}(\mathbf{x})$	
Link_Field	$L_{\mu}(\mathbf{x})$	$\overline{\mathcal{D}}_{\mu}^{(+)}S(\mathbf{x})$	$\mathcal{D}_{\nu}^{(-)}P_{\mu\nu}(\mathbf{x})$
Plaquette_Field	$P_{\mu\nu}(\mathbf{x})$	$\mathcal{D}^{(+)}_{\mu}L_{ u}(\mathbf{x})$	$\overline{\mathcal{D}}_{\rho}^{(-)}B_{\mu\nu\rho}(\mathbf{x})$
Body_Field	$B_{\rho\mu\nu}(\mathbf{x})$	$\overline{\mathcal{D}}_{\rho}^{(+)}P_{\mu\nu}(\mathbf{x})$	

As an instructive example let us look at the coding details of the Link\_Field class. In figure 5 we show how the Link\_Field class is defined along with overloading of basic operators such as '+' and '-'.

We look at the structure of the fermionic term  $\eta \overline{\mathcal{D}}_{\mu} \psi_{\mu}$  on the lattice and the structure of the corresponding fermionic operator in the code. On the lattice this fermionic term takes the form

$$\eta \overline{\mathcal{D}}_{\mu} \psi_{\mu} \rightarrow \frac{1}{2} \Big[ \eta(\mathbf{x}) \overline{\mathcal{D}}_{\mu}^{(-)} \psi_{\mu}(\mathbf{x}) + \psi_{\mu}(\mathbf{x}) \overline{\mathcal{D}}_{\mu}^{(+)} \eta(\mathbf{x}) \Big] \\ = \frac{1}{2} \Big[ \eta^{a}(\mathbf{x}) T^{a} \overline{\mathcal{D}}_{\mu}^{(-)} T^{b} \psi_{\mu}^{b}(\mathbf{x}) + \psi_{\mu}^{b}(\mathbf{x}) T^{b} \overline{\mathcal{D}}_{\mu}^{(+)} T^{a} \eta^{a}(\mathbf{x}) \Big] , \quad (62)$$

where  $T^a$  are the generators of the gauge group.

On expanding the lattice covariant difference operators we have

$$\eta \overline{\mathcal{D}}_{\mu} \psi_{\mu} \rightarrow \frac{1}{2} \Big[ \eta^{a}(\mathbf{x}) T^{a} \Big( T^{b} \psi^{b}_{\mu}(\mathbf{x}) \mathcal{U}^{\dagger}_{\mu}(\mathbf{x}) - \mathcal{U}^{\dagger}_{\mu}(\mathbf{x} - \widehat{\boldsymbol{e}}_{\mu}) T^{b} \psi^{b}_{\mu}(\mathbf{x} - \widehat{\boldsymbol{e}}_{\mu}) \Big) \\ + \psi^{b}_{\mu}(\mathbf{x}) T^{b} \Big( T^{a} \eta^{a}(\mathbf{x} + \widehat{\boldsymbol{e}}_{\mu}) \mathcal{U}^{\dagger}_{\mu}(\mathbf{x}) - \mathcal{U}^{\dagger}_{\mu}(\mathbf{x}) T^{a} \eta^{a}(\mathbf{x}) \Big) \Big] \\ = \frac{1}{2} \Big[ \eta^{a}(\mathbf{x}) \Big( T^{a} T^{b} \mathcal{U}^{\dagger}_{\mu}(\mathbf{x}) \Big) \psi^{b}_{\mu}(\mathbf{x}) - \eta^{a}(\mathbf{x}) \Big( T^{a} \mathcal{U}^{\dagger}_{\mu}(\mathbf{x} - \widehat{\boldsymbol{e}}_{\mu}) T^{b} \Big) \psi^{b}_{\mu}(\mathbf{x} - \widehat{\boldsymbol{e}}_{\mu}) \Big) \\ + \psi^{b}_{\mu}(\mathbf{x}) \Big( T^{b} T^{a} \mathcal{U}^{\dagger}_{\mu}(\mathbf{x}) \Big) \eta^{a}(\mathbf{x} + \widehat{\boldsymbol{e}}_{\mu}) - \psi^{b}_{\mu}(\mathbf{x}) \Big( T^{b} \mathcal{U}^{\dagger}_{\mu}(\mathbf{x}) T^{a} \Big) \eta^{a}(\mathbf{x}) \Big) \Big] . \quad (63)$$

In the code we compute the combination  $\operatorname{Tr}(T^a\mathcal{U}_{\mu}(\mathbf{x})T^b)$  as  $V_{\mu}(\mathbf{x})^{ab}$  and store it as the object Adjoint\_Link\_Field. It is this field that is passed into the functions that require the action of the twisted fermion operator in the inverter. Explicitly, the contribution to the operator coming from the term  $\operatorname{Tr}\eta\overline{\mathcal{D}}_{\mu}\psi_{\mu}$  in the action takes the following form in the code:

#### 5. Numerical results

In this section we provide some numerical results obtained through the recent simulations of the two-dimensional  $\mathcal{N} = 2$  lattice SYM theory [50].

The results we show in this section were obtained using the standard Wilson prescription for the parametrization of the complexified gauge fields  $\mathcal{A}_{\mu}(x)$  on the lattice. The continuum fields  $\mathcal{A}_{a}(x)$  are mapped to link fields  $\mathcal{U}_{a}(\mathbf{n})$  living on the link between  $\mathbf{n}$  and in  $\mathbf{n} + \hat{\boldsymbol{\mu}}_{a}$  through the mapping:

$$\mathcal{U}_a(\mathbf{n}) = e^{\mathcal{A}_a(\mathbf{n})} , \qquad (64)$$

where  $\mathcal{A}_a(\mathbf{n}) = \sum_{i=1}^{N_G} \mathcal{A}_a^i T^i$  where  $T^i = 1 \dots N_G$  are the anti-hermitian generators of a U(N) group. The resultant gauge links take their values in  $GL(N, \mathbb{C})$ . Notice though that in spite of the appearance of a complex connection the theory only possesses the usual U(N) gauge symmetry. We call this realization of the bosonic links the group or exponential parametrization<sup>10</sup> to distinguish it from another realization of the bosonic links - the linear parametrization,  $\mathcal{U}_a(\mathbf{n}) = \mathbb{I} + \mathcal{A}_a(\mathbf{n})$  - used in orbifold constructions of the lattice SYM theories. Simulations with linear gauge links are also possible and indeed have been investigated in [50].

 $<sup>^{10} \</sup>rm Notice$  that our lattice gauge fields are dimensionless and hence contain an implicit factor of the lattice spacing a.

#### 5.1. Eigenvalues of scalars

The requirement that the lattice theory target the continuum theory as the lattice spacing is sent to zero demands vanishing of the fluctuations of all lattice fields and *in particular the fluctuations of the trace part of the scalar field*  $B_a^0$ . Given the absence of any classical potential guaranteeing this, we find that it is necessary to add a suitable gauge-invariant potential to the lattice theory to ensure this condition holds<sup>11</sup>. In principle, once this mode is regulated one can examine whether this potential can be sent to zero in the continuum limit.

We have added a simple potential term of the following form to regulate the trace mode in the simulations:

$$S_M = \mu^2 \sum_x \left(\frac{1}{N} \operatorname{Tr}(\mathcal{U}_a^{\dagger}(x)\mathcal{U}_a(x)) - 1\right)^2 .$$
(65)

This term gives a mass only to the trace mode of the scalars to leading order in the lattice spacing

$$S_M \approx \mu^2 \sum_x \left[ \text{Tr} \left( e^{2iB_a + \dots} - 1 \right) \right]^2 = \left( \frac{2\mu}{N\sqrt{N}} \right)^2 \sum_x (B_a^0)^2 + \dots$$
 (66)

Since this U(1) scalar sector decouples in the naive continuum limit this should not break the supersymmetry of the remaining SU(N) sector for small enough lattice spacing.

In the C++ code the mass term (65) is implemented using

#### (1.0/NCOLOR)\*Tr(Udag.get(x,mu)\*U.get(x,mu)).real()-1.0

in action.cpp. The U(1) mass coefficient  $\mu$  is denoted by the parameter BMASS.

We rescale all lattice fields by powers of the lattice spacing to make them dimensionless. This leads to an overall dimensionless coupling parameter of the form  $N/(2\lambda a^2)$ , where  $a = \beta/T$  is the lattice spacing,  $\beta$  is the physical extent of the lattice in the Euclidean time direction and T is the number of lattice sites in the time-direction. The coupling  $\lambda = g^2 N$  is the usual 't Hooft parameter. Thus, the lattice coupling

$$\kappa = \frac{NT^2}{2\lambda\beta^2} , \qquad (67)$$

for the symmetric two-dimensional lattice where the spatial length L = T. Note that  $\lambda\beta^2$  is the dimensionless physical 't Hooft coupling measured in units of the area. In these two dimensional simulations, the continuum limit can be approached by fixing  $t = \lambda\beta^2$  and N, and increasing the number of lattice points  $L \to \infty$ . We have taken three different values for this coupling t = 0.5, 1.0, 2.0and lattice sizes ranging from  $L = 2, \cdots, 12$ . In fig. 6 we show the average

<sup>&</sup>lt;sup>11</sup>It was precisely this requirement that led to a truncation of the U(N) symmetry to SU(N) in the original simulations of these theories corresponding to a delta function potential for the U(1) part of the field [14].



Figure 6: Plot showing the average scalar eigenvalue versus the lattice size L in the twodimensional Q = 4 theory.

scalar eigenvalue given by  $\mathcal{U}_a^{\dagger}\mathcal{U}_a - I$  for the  $\mathcal{Q} = 4$  model as a function of the lattice size L. This figure confirms that as  $L \to \infty$  we are indeed approaching a continuum limit since the scalar eigenvalues (which contain a factor of a to render them dimensionless) are driven to zero.

#### 5.2. Pfaffian phase/sign problems

The models we have discussed may encounter an additional difficulty in the context of simulation - the fermionic sign problem. After integration over the fermions the effective bosonic action picks up a contribution from the logarithm of the fermionic Pfaffian Pf(M) which is not necessarily real. Indeed for the supersymmetric lattice constructions we described above, M at non zero lattice spacing is a complex operator and one might worry that the resulting Pfaffian could exhibit a fluctuating phase  $e^{i\alpha}$ . Since Monte Carlo simulations must necessarily be performed with a positive definite measure the only way to incorporate this phase is through a re-weighting procedure which folds the phase in with the observables of the theory. Expectation values of observables derived from such simulations can then suffer huge statistical errors which swamp the signal rendering the Monte Carlo techniques effectively useless.

In fig. 7 we show results for  $\langle |\sin(\alpha)| \rangle$  as a function of L for the Q = 4 model with gauge group U(2). Three values of  $t = \lambda \beta^2$  are shown in each plot but the behavior is qualitatively similar for all t. We have used the mass parameter controlling the U(1) mode as BMASS = 1. These numerical results show that while this model appears to suffer from a severe sign problem for coarse lattices these effects disappear as the lattice is refined and the phase fluctuations are driven to zero as the continuum limit is taken. This picture is consistent with



Figure 7: Plot showing the average of the sin of the Pfaffian phase  $\alpha$  against the lattice size L in the Q = 4 lattice SYM with gauge group U(2) and exponential representation for the gauge links.

both the old results of [14] and the more recent work in  $[51]^{12}$ .

# 5.3. Restoration of supersymmetry

The topological nature of the twisted theory formulated on a torus with periodic boundary conditions can be used to show that the partition function of the lattice model is actually independent of the coupling constant. Thus derivatives of the partition function with respect to the coupling constant such as the expectation value of the action must vanish. Since the fermions enter only quadratically their contribution can be evaluated simply using a scaling argument and thence a simple expression derived for the expectation value of the bosonic action. Thus measurements of  $\langle S_B(\mathcal{U}, \overline{\mathcal{U}}) \rangle$  provide us with a check that the scalar supersymmetry has indeed been implemented correctly in our codes. Actually, since in practice we use supersymmetry breaking (thermal) boundary conditions (and also employ a susy breaking potential for the scalar U(1) mode) to do simulations, measuring this quantity provides some insight into the magnitude of supersymmetry breaking effects in the theory.

In the case of two-dimensional Q = 4 theory, we have the expression for the mean action

$$\langle S \rangle = -\frac{\partial \ln Z}{\partial \kappa} = \langle Q \Lambda \rangle = 0 , \qquad (68)$$

where  $\kappa$  is the coupling constant of the twisted action and the last equality follows from the Q-exact nature of the twisted theory and shows that the vanishing

<sup>&</sup>lt;sup>12</sup>The results reported in [14] actually used the group SU(2) but we have checked by explicit simulation that similar results are obtained with large  $\mu$  using U(2) and an exponential parametrization for the links.



Figure 8: Plot showing the average bosonic action  $\langle \kappa(S_B + S_M) \rangle$  on the lattice against the lattice size L in the Q = 4 lattice SYM with gauge group U(2) and exponential parametrization for the gauge links. The thick solid line corresponds to the exact value of the bosonic action.

mean action can be thought of as arising as a consequence of a simple Q-Ward identity.

If we integrate out the twisted fermions and the auxiliary field d we find the following expression for the partition function of the two-dimensional Q = 4 theory

$$Z = \kappa^{4N_G V/2} \kappa^{-N_G V/2} \int D\mathcal{U} D\overline{\mathcal{U}} e^{-\kappa S_B(\mathcal{U},\overline{\mathcal{U}})} \det(M(\mathcal{U},\overline{\mathcal{U}})) , \qquad (69)$$

where  $N_G$  is the number of generators of the gauge group and V is the number of lattice points. The first prefactor arises from the fermion integration and the second derives from the Gaussian integration over the auxiliary field. From this we find the following condition on the mean bosonic action as a consequence of the scalar supersymmetry Q:

$$\langle \kappa S_B \rangle = \frac{3}{2} N_G V \ . \tag{70}$$

In figure 8 we show the mean bosonic action on the lattice against the lattice size L. The thick solid line represents the exact value of the bosonic action given in 70. Clearly the lattice measurements approach the exact result for sufficiently small lattice spacing. The deviations that are visible are presumably related to the fact that we have a sign problem (these measurements do *not* incorporate reweighting) for small L and the simulations are also conducted at non zero temperature. We have shown that the sign problem disappears in the continuum limit which is consistent with the mucgh better agreement at large L. To recover the true zero temperature result requires in principle that we extrapolate our measurements to  $t \to \infty$  after taking the thermodynamic limit.

#### 6. Conclusions

In this paper we have described in some detail the construction of an object oriented code suitable for the simulation of a recently discovered class of lattice field theory possessing exact supersymmetry. The cases of Q = 4, 8, 16 supercharges in two, three and four dimensions are all covered in detail. The structure of the problem requires the construction of unusual data structures for representing the fermions which is the primary difference between the code described here and more conventional codes suitable for simulating QCD. Nevertheless the basic algorithms employed (RHMC and multimass CG solvers) are borrowed directly from lattice QCD and adapted to the problem at hand. We verify the correctness of the resultant code by showing results from simulations of the two dimensional model. Acceleration of the code can be achieved by offloading the linear solver calculation to a GPU card - we refer the reader to [52] for details. It is also possible to parallelize the code with suitable distributed libraries layered over MPI [53] and work in both these directions is ongoing.

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