Progress using generalized lattice Dirac operators to parametrize the Fixed-Point QCD action

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We report on an ongoing project to parametrize the Fixed-Point Dirac operator for massless quarks, using a very general construction which has arbitrarily many fermion offsets and gauge paths, the complete Clifford algebra and satisfies all required symmetries. Optimizing a specific construction with hypercubic fermion offsets, we present some preliminary results.

1. Motivation for improved fermionic actions

There are many reasons to seek an improved lattice Dirac operator. The most commonly used one, the Wilson Dirac operator, has a number of problems. Chiral symmetry, an essential element of QCD, is broken explicitly by a term which removes the fermion-doublers and so the pion is not massless for zero quark mass. The pion can be tuned massless by varying the hopping parameter. However, this does not remove other problems, such as the mixing of operators in different chiral representations, which makes the extraction of chiral matrix elements difficult. There are also problems measuring chiral quantities such as the quark condensate and zero modes of the Dirac operator and connecting these to the topology of the gauge fields, due to, among other things, topological defects and exceptional configurations. In addition, the Wilson Dirac operator has large lattice artifacts.

A solution to problems of chirality has been proposed by Ginsparg and Wilson\textsuperscript{[1]}: a lattice Dirac operator which satisfies

\[
\{\gamma_5, D^{-1}\} = 2 aR \gamma_5, \tag{1}
\]

where \(R\) is any local function which commutes with \(\gamma_5\) and \(a\) is the lattice spacing, was expected to define a lattice theory with the same chiral properties as the continuum theory. Unfortunately, no solution to this relation was found and the idea was abandoned. The first lattice regularization of fermions with chiral symmetry, the Domain Wall fermions\textsuperscript{[2]} and the related Overlap construction\textsuperscript{[3]}, followed a different path and seemed to be unrelated to the Ginsparg-Wilson (GW) relation.

Following the observation that the Fixed-Point Dirac operator satisfies the GW relation\textsuperscript{[4]}, the interest turned to this general formulation again. The GW relation turned out to be a powerful theoretical tool: it implies an index theorem on the lattice\textsuperscript{[5]} and all the chiral properties of the formal continuum theory\textsuperscript{[6]}. This last feature became trivial after it was recognized that an exact chiral symmetry transformation follows from eq.(1)\textsuperscript{[7]}. The observation that the Overlap Dirac operator satisfies the GW relation connected the Domain Wall approach to this general formulation\textsuperscript{[8]}. The progress in vector chiral symmetry was followed by a breakthrough in the formulation of regularized chiral gauge theories also\textsuperscript{[8]}.

All these developments have led to much recent activity on the theoretical understanding of lattice chiral symmetry\textsuperscript{[9,10]} and on constructing improved lattice Dirac operators which approximately satisfy the GW relation\textsuperscript{[11,12]}. At the same time, detailed tests and the first large-scale simulations with the simplest version of Domain...
Wall and Overlap Dirac operators demonstrated the power and difficulties of working with chirally symmetric QCD actions \[\square\].

2. General lattice Dirac operators

Before we explain our approach to the parametrization of the Fixed-Point Dirac operator we briefly discuss the structure of general Dirac operators which satisfy the basic symmetries on the lattice. This will make clear what kind of lattice operators can be used in the parametrization of the Fixed-Point Dirac operator or in any other parametrization of a Dirac operator. A more detailed discussion of these issues is given in \[\square\]. A general gauge covariant lattice operator with color, space and Dirac indices can be written as:

\[
D = \sum_A \Gamma_A \sum_l c(\Gamma_A, l) \hat{U}(l),
\]

where the \(\Gamma_A\) are elements of the Clifford algebra basis which we define as \(\Gamma = 1, \gamma_\mu, i\sigma_{\mu\nu}, \gamma_5, \gamma_\mu\gamma_5\), \(l\) denotes a path, \(\hat{U}(l)\) the product of the link matrices along this path and \(c(\Gamma_A, l)\) is the coupling for the given path and Clifford algebra element.

The basic symmetries of the Dirac operator, which are gauge symmetry, \(\gamma_5\)-hermiticity, charge conjugation, hypercubic rotations and reflections, impose the following restrictions on eq.(3):

- Translation invariance requires that the Dirac operator \(D(n, n + r)\) connecting lattice sites \(n\) and \(n + r\) depends on \(n\) only through the \(n\)-dependence of the gauge field, i.e. the couplings \(c(\Gamma_A, l)\) are constants or gauge invariant functions of gauge fields, respecting locality and invariance under the symmetry transformations.

- \(\gamma_5\)-hermiticity and charge conjugation together imply that the couplings \(c(\Gamma_A, l)\) for our choice of the Clifford algebra basis are real. Further, from hermiticity it follows that the path \(l\) and the opposite path \(\bar{l}\) (or equivalently, \(\hat{U}(l)\) and \(\hat{U}(l)^\dagger\)) should enter in the combination

\[
\Gamma \left( \hat{U}(l) + \epsilon_\Gamma \hat{U}(l)^\dagger \right),
\]

where the sign \(\epsilon_\Gamma\) is defined by \(\gamma_5\Gamma^\dagger \gamma_5 = \epsilon_\Gamma \Gamma\).

- Permutations and reflections of the coordinate axes (hypercubic rotations) imply that for a given path \(l_0\) a whole class of paths belongs to the Dirac operator. These paths are related to \(l_0\) by all the \(16 \times 24 = 384\) reflections and permutations of the coordinate axes. Under such a symmetry transformation \(\alpha = 1, \ldots, 384\) the Clifford algebra element \(\Gamma_0\) associated with \(l_0\) generally transforms into \(\Gamma^{(\alpha)}\). Furthermore the sign of the couplings may change, whereas their absolute value remains unchanged.

A Dirac operator satisfying all the basic symmetries can be written as

\[
D = \sum_{\Gamma_0, l_0} c(\Gamma_0, l_0) \sum_\alpha O^{(\alpha)}
\]

where the sum runs over a set of reference paths defined by \(\Gamma_0\) and \(l_0\) as well as over all the symmetry transformations \(\alpha\) defined by the group of permutations and reflections of the coordinate axes.

It is quite natural to include the full Clifford algebra in the Dirac operator. The Wilson operator already contains \(1\) and \(\gamma_\mu\), the \(O(\alpha)\) Symmzink condition involves \(\sigma_{\mu\nu}\) and the topological charge is proportional to \(\text{Tr}(\gamma_5 D)\), which is zero unless \(D\) contains \(\gamma_5\). Furthermore, for \(\gamma_5\)-hermitian Dirac operators, the Ginsparg-Wilson relation \(\square\) can be written as

\[
D + D^\dagger = 2 \alpha D^\dagger RD,
\]

which can only be satisfied if \(D\) contains the complete Clifford algebra.

3. Efficient implementation of general Dirac operators

On first appearances one might think that it is not feasible to calculate such a general Dirac operator which has many different couplings, where every coupling might contain as many as \(768\) paths. But one has to keep in mind that the calculation of propagators for small quark masses
needs several hundreds or even thousands of conjugate gradient steps and therefore one can afford to spend some time to precalculate and store the whole Dirac operator before one starts the calculation of the propagator. On top of this there are two reasons why the building of general operators can be done in a very efficient way:

- There are a lot of paths which are invariant under certain subgroups of the reflections and permutations which reduces the number of terms significantly and in some case even leads to a cancellation of certain terms because they have relative minus signs.

- A less trivial fact is that the sum of paths for many couplings can be factorized in an efficient way, i.e. that such large sums of many paths can be written as a product of smaller sums of fewer paths.

As an example we consider a nearest neighbour coupling with \( \Gamma_0 = \gamma_5 \) and generating path \( l_0 = [2, 1, -2, 3, 4, -3, -4] \), where a path \( l \) is a sequence of steps in the \( \pm \mu \) direction. All the paths of this coupling can be written in the following compact way:

\[
\gamma_5 \sum_{\mu \nu \rho \sigma} \epsilon_{\mu \nu \rho \sigma} (S_{\mu \nu} P_{\rho \sigma} + P_{\rho \sigma} S_{\mu \nu} + \text{h.c.}) ,
\]

where the color matrices \( S_{\mu \nu} \) and \( P_{\rho \sigma} \) are certain combinations of staples or plaquettes, respectively. When all the plaquettes and staples and the most frequent combinations, e.g. \( P_{\rho \sigma} \), are pre-calculated then operators as in eq. (6) can be calculated very quickly. As an illustration of this we consider one of our parametrizations of the Fixed-Point Dirac operator. It has 39 couplings in total, at least one per offset on the 1-hypercube and per type of Clifford algebra element. Building this operator takes roughly 15 times as long as to multiply the operator with a vector and therefore it is a very small fraction of the time used to perform a calculation of one propagator.

The basic operation required to calculate propagators or eigenvalues is the multiplication of the Dirac operator times a vector. For a Dirac operator with hypercubic fermion offsets which contains the complete Clifford algebra, the matrix times vector multiplication is roughly 40 times more expensive than for the Wilson Dirac operator.

In \cite{14}, we have included a MAPLE code which, given an input path \( l \) and any Clifford algebra element \( \Gamma \), gives all of the paths \( l^{(\alpha)} \) and algebra elements \( \Gamma^{(\alpha)} \) generated by all permutations and reflections of the coordinate axes. This can be used by anyone who wishes to use a very general lattice Dirac operator, independently of how this operator is optimized.

4. Fixed-Point improved actions

The Fixed-Point method of improving lattice actions is inspired by the Renormalization Group flow of asymptotically-free theories \cite{16}. Consider a lattice action which contains all possible interactions. The Renormalization Group is defined by some blocking function which averages over the fields to produce a new action on a coarser lattice with fewer fields. The new action typically has different couplings from the original action and so we can imagine the blocking step as a flow in the coupling parameter space. Infinitely many blocking steps give the complete Renormalization Group (RG) trajectory. In Figure 1, we show the RG trajectory for QCD with massless quarks. The Fixed-Point (FP) has the property that the couplings are reproduced after a blocking step. For asymptotically-free theories, the Fixed-Point is on the surface of vanishing coupling \( g = 0 \).

If one starts on this surface, the RG trajectory flows quickly to the Fixed-Point. If one starts close to this surface at some small coupling \( g \) (i.e. small lattice spacing \( a \)), the RG trajectory flows quickly towards the Fixed-Point and then flows away from it. Starting on the RG trajectory with arbitrarily fine lattices with arbitrarily small lattice artifacts, one can reach any point on the trajectory by making sufficiently many blocking steps. All actions on the trajectory describe the same physics. The physical observables of the continuum quantum theory are identical to those of any lattice quantum theory on the RG trajectory, independently of the lattice coarseness. Such lattice actions are said to be quantum perfect. The Fixed-Point action is an approximation
to the RG trajectory for small couplings $g$ and is classically perfect, i.e. it completely describes the continuum classical theory without discretization errors.

Fixed-Point actions have many desirable features. By closely approximating the RG trajectory, they are expected to have much reduced quantum lattice artifacts. They can be optimized for locality. The Fixed-Point Dirac operator satisfies the Ginsparg-Wilson relation and so has good chiral behavior. The Fixed-Point QCD action has well-defined topology and satisfies the index theorem on the lattice. Although more expensive than standard actions, studies of other models have shown that practical Fixed-Point actions can be constructed and used [17].

5. Free Fixed-Point fermions

We first consider free massless fermions. Because the fermionic action is quadratic in the fermionic fields, the Renormalization Group step for the fermionic fields amounts to Gaussian integration, which can be done exactly. The blocking step connects the Dirac operator on the fine (F) and coarse (C) lattices by

$$D_C^{-1} = \frac{1}{\kappa} + \Omega \, D_F^{-1} \, \Omega^\dagger,$$

provided $D_F$ has no zero modes, where $\kappa$ is an optimizable free parameter of the blocking and $\Omega$ is the blocking function used to integrate out the fine fields to produce the coarse fields. The FP Dirac operator is reproduced under the blocking step i.e. $D_C = D_F = D_{FP}$. For free fermions, this equation can be solved exactly analytically. The FP Dirac operator is local, i.e. the couplings fall off exponentially with distance, and the rate of fall off can be maximized by varying $\kappa$. However, $D_{FP}$ contains infinitely many couplings. For practicality, $D_{FP}$ is approximated with an ultra-local operator, for which each point is only coupled to its neighbours on the hypercube. In Figure 2, we see the exact $D_{FP}$ reproduces exactly the continuum dispersion relation, while the approximate FP Dirac operator has much smaller discretization errors than the Wilson operator. The unphysical branches in the approximate $D_{FP}$ occur at large momenta and only have a small effect.
The Ginsparg-Wilson relation eq.(4) is a constraint on \( \{\gamma_5, D^{-1}\} \). The FP equation (7) connects the propagators \( D^{-1} \) on the coarse and fine lattices. Combining these equations gives

\[
R_C = \frac{1}{\kappa} + \Omega R_F \Omega^\dagger, \tag{8}
\]

and at the Fixed-Point, \( R_C = R_F = R_{FP} \). For free fermions, this equation can also be solved exactly analytically. Choosing a symmetric overlapping block transformation \( \Omega \) with a scale factor 2 averaging over hypercubes [8], the exact \( R_{FP} \) is ultra-local and has only hypercubic couplings — no approximation for practicality is required. The block transformation \( \Omega \) determines \( R \). With other methods to build a Dirac operator satisfying the Ginsparg-Wilson relation, for example the Overlap construction, \( R \) is unconstrained and typically \( R = \frac{1}{2} \).

Defining a rescaled Dirac operator \( d = \sqrt{2R} D \sqrt{2R} \), the Ginsparg-Wilson relation can be written (with lattice spacing \( a = 1 \))

\[
d + d^\dagger = d^\dagger d, \tag{9}
\]

i.e. the eigenvalues of \( d \) lie on a circle of radius 1 centred at \((1, 0)\). Using \( R_{FP} \) and the hypercubic approximation of \( D_{FP} \), we show the eigenvalue spectrum of \( d \) in Figure 3. It lies almost exactly on the circle, indicating that the hypercubic truncation has only slightly affected the Ginsparg-Wilson property.

6. Parametrization of the QCD FP Dirac operator

To parametrize the QCD FP Dirac operator \( D_{FP} \) for massless quarks, we use a general Dirac operator as defined in eq.(4) with all the couplings of the 1-hypercube and all elements of the Clifford algebra. The gauge invariant functions we use as couplings of \( D_{FP} \) are polynomials in local fluctuations of the gauge fields. Furthermore we include the possibility to smear the gauge fields and to project them back to SU(3), i.e. we are using so called fat links. We use the new parametrization of the FP gauge action [19] which also makes use of fat gauge links.

The QCD FP action is also quadratic in the fermion fields and the Renormalization Group step can again be done analytically. The QCD FP equation is the generalization of the free equation (7) given by including gauge fields. In case \( D_F \) has zero modes, the QCD FP equation is most conveniently written as

\[
D_C(V) = \kappa 1 - \kappa^2 \Omega(U)[D_F(U) + \kappa \Omega^\dagger(U)\Omega(U)]^{-1} \Omega^\dagger(U), \tag{10}
\]

where \( \kappa \) is an optimizable free parameter of the block transformation and \( U \) and \( V \) are the gauge fields on the fine and coarse lattice, respectively. They are related through the FP equation of the pure SU(3) gauge theory

\[
S_{FP}^C(V) = \min_{\{U\}} (S_{FP}^F(U) + T(U, V)), \tag{11}
\]

where \( S_{FP}^C \) is the FP action of the pure SU(3) gauge theory and \( T(U, V) \) is the blocking kernel of the block transformation. As the fluctuations of the gauge fields on the fine lattice are much smaller than those of the coarse gauge fields, the Dirac operator used on the fine lattice has to have good chiral properties on gauge fields with small
fluctuations. This however is by far easier than to have a Dirac operator with good chiral properties on gauge fields with large fluctuations. An important fact for the parametrization of the FP Dirac operator is that eq. (14) can also be given in terms of the propagators

\[ D_C^{-1}(V) = \frac{1}{\kappa} + \Omega(U) D_F^{-1}(U) \Omega(U), \]

(12)
as long as \( D_F \) has no zero modes. In contrast to eq. (10), the equation for the propagator gives much more weight to the small physical modes of the Dirac operator and can therefore be used to improve the properties of the small modes of the parametrized FP Dirac operator.

The parametrization is an iterative procedure. We first start at a large value of \( \beta \), generate thermal coarse gauge configurations \( V \) with the FP gauge action and determine the corresponding fine configurations \( U \) via minimization as in eq. (11). Using the free FP Dirac operator on the fine configurations (which have very small fluctuations), \( D_C(V) \) and \( D_C^{-1}(V) \) are calculated from eqs. (11) and (12). The couplings of the parametrized Dirac operator \( D_{\text{par}} \) are determined by minimizing the following \( \chi^2 \)-function:

\[ \chi^2 = \sum ||D_{\text{par}}v - D_Cv||^2 + \lambda \sum ||D_{\text{par}}^{-1}v - D_C^{-1}v||^2, \]

(13)

where the sum runs over a number of random vectors \( v \) on different configurations and \( \lambda \) is a weighting factor. The use of vectors for the calculation of a \( \chi^2 \) function for \( D_{\text{par}} \) is mandatory because the definition of \( D_C \) requires a matrix inversion which we can afford only for a limited number of vectors. The minimization of the \( \chi^2 \) yields a parametrized FP Dirac operator \( D_{\text{par}}(V) \) which has good chiral properties over a larger range of gauge couplings than the initial truncated free FP Dirac operator.

The fitted parametrized operator \( D_{\text{par}} \) is now used on fine configurations \( U' \), determined via minimization from coarse configurations \( V' \) generated thermally at a smaller value of \( \beta \). Minimizing the \( \chi^2 \) in eq. (13) again gives \( D_{\text{par}}(V') \) which performs well on an even larger range of gauge couplings. The whole procedure is repeated until we reach \( \beta = 3.0 \) which corresponds to \( \beta_{\text{Wilson}} \approx 5.75 \). During this procedure we keep leading terms in the naive continuum limit fixed such that the tree level mass is zero, the \( O(a) \) Symanzik condition is fulfilled, the dispersion relation starts with slope 1 and the normalization of the topological charge is correct. Furthermore we fix the free field limit such that we recover the truncated free FP operator on the trivial gauge configuration.

In order to parametrize the operator \( R \) in eq. (8) we proceed in a similar way as for the Dirac operator. We also use a general operator with fat links and fluctuation polynomials. The parametrization of \( R \) is however simpler as it is trivial in Dirac space and therefore contains a smaller number of operators. In contrast to the equation for the block transformation of \( D_{FP} \) the corresponding equation for \( R \) in eq. (8) contains no inversion and therefore the \( \chi^2 \)-function which we minimize in order to find the optimal parametrization of \( R_{\text{par}} \) can be defined as

\[ \chi^2 = ||R_{\text{par}} - R_C||^2, \]

(14)

where the norm here is the matrix norm \( ||A||^2 = \sum_{ij} ||a_{ij}||^2 \).

7. Preliminary results

We have some preliminary results for the parametrized QCD FP Dirac operator. In Figure 7 we show the spectrum of exact eigenvalues of \( d = \sqrt{2}R \) \( D \) at \( \beta = 3.0 \), i.e. \( \beta_{\text{Wilson}} \approx 5.75 \), corresponding to a lattice spacing of \( a \approx 0.16 \) fm. We show all the eigenvalues on a \( 4^4 \) volume (crosses) and those closest to the origin on an \( 8^4 \) volume (circles). We see that the spectrum lies quite close to the Ginsparg-Wilson circle, with a small additive mass renormalization. This is evidence that the parametrization is sufficiently rich to reproduce well the chiral Fixed-Point properties.

In order to measure hadron masses, one needs to calculate the quark propagators. The quark propagators are determined by solving the equation \( X = D^{-1}\eta \) for some source vector \( \eta \). We have measured the accuracy \( \epsilon_k \) in calculating the inverse, \( \epsilon_k = ||D(D^{-1}\eta)_k - \eta|| \), after \( k \) conju-
gate gradient steps, i.e., how many times $\eta$ is multiplied by $D$ in calculating $D^{-1}\eta$. To achieve a given accuracy, we find that the parametrized FP Dirac operator requires roughly 3 times fewer steps than the unpreconditioned Wilson operator corresponding to the same effective pion mass for the same gauge configuration. This reduces the overhead of $D_{\text{par}}$ in production runs.

The chiral properties of a Dirac operator are improved by using the Overlap construction. Given some input Dirac operator $D_0$, a Dirac operator which satisfies the Ginsparg-Wilson relation is given by

$$D_{\text{OV}} = 1 - \frac{A}{\sqrt{A^\dagger A}}, \quad A = 1 - D_0. \quad (15)$$

If the input operator already satisfies the Ginsparg-Wilson relation, then $A^\dagger A = 1$ and $D_{\text{OV}} = D_0$. The inverse square root is calculated by some expansion in $A^\dagger A$. How quickly the expansion converges is determined by the smallest and largest eigenvalues of $A^\dagger A$, which tells us how far the input operator is from satisfying the Ginsparg-Wilson relation.

In Figure 5, we plot the 10 smallest eigenvalues of $A^\dagger A$ at $\beta = 3.4$ ($\beta_{\text{Wilson}} \approx 5.95$) for the parametrized FP (squares) and Wilson (crosses) Dirac operators for 30 configurations.

The parametrized FP operator $d$ approximately satisfies the Ginsparg-Wilson relation and the inverse square root can be determined accurately by, for example, a Legendre expansion with only a few terms, which would very much improve the already good chiral behavior of $d$. The expansion converges faster by projecting out the smallest eigenvalues, which are treated exactly. Using $d$, we see $A^\dagger A$ has few small eigenvalues and so the projection can be done quite cheaply. In contrast, using $D_{\text{Wilson}}$ to construct $A$, most of the eigenvalues of $A^\dagger A$ are far from 1 and very expensive expansions with up to hundreds of terms are required to determine the inverse square root. There are also more very small eigenvalues to be
fixed point Wilson

Figure 6. Histogram of number of multiplications to find 10 smallest eigenvalues of $A^\dagger A$ for all configurations plotted in Figure 5. Using $d$ in the Overlap construction, fewer small eigenvalues need be treated exactly and these can be determined with fewer multiplications than are necessary using $D_{\text{Wilson}}$.

8. Conclusions

The project of parametrizing the QCD FP Dirac operator is ongoing. Preliminary results show that the parametrization achieved so far gives a Dirac operator which satisfies the Ginsparg-Wilson relation quite well with a small additive mass renormalization. Although a matrix vector multiplication with $D_{\text{par}}$ is roughly 40 times more expensive than with $D_{\text{Wilson}}$, we see that calculating eigenvalues and propagators converges much faster. The chiral properties of a Dirac operator are greatly improved by using it as input for the Overlap construction. As $D_{\text{par}}$ is already quite close to satisfying the Ginsparg-Wilson relation, the Overlap construction using $D_{\text{par}}$ is comparable in cost to using $D_{\text{Wilson}}$.

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