Constructing Improved Overlap Fermions in QCD

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We describe an explicit construction of approximate Ginsparg-Wilson fermions for QCD. We use ingredients of perfect action origin, and further elements. The spectrum of the lattice Dirac operator reveals the quality of the approximation. We focus on $\beta = 6$ for optimisation. Such fermions are intended to be inserted into the overlap formula. Hence we also test the speed of convergence under polynomial evaluation of the overlap formula.

1. Introduction

If a lattice Dirac operator $D$ obeys the Ginsparg-Wilson relation (GWR) \cite{1}
\[ \{D_{x,y}, \gamma_5\} = 2(D\gamma_5 RD)_{x,y}, \]  
then it reproduces correctly the physical properties related to chirality \cite{2}. In particular, a GW fermion has a chiral symmetry, which is lattice modified but exact \cite{3}.

The kernel $R$ must be local, and $\{R, \gamma_5\} \neq 0$. For simplicity we assume
\[ R_{x,y} = \frac{1}{2\mu} \delta_{x,y} (\mu > 0), \text{ and } D^\dagger = \gamma_5 D \gamma_5. \]  
Then the spectrum of $D$ is situated on a circle in the complex plane: it is the circle through 0 with centre and radius $\mu$.

Classically perfect fermion actions solve the GWR \cite{2} and their scaling is excellent, but they are hard to construct. They were applied successfully in the Schwinger model \cite{4,5}, and the tedious work in $d = 4$ is still in progress \cite{6}.

There are, however, many more GW fermions: starting from almost any sensible lattice Dirac operator $D_0$ (local, free of doublers etc.) we can generate a solution to the GWR by means of the overlap formula
\[ D_{\text{ov}} = \mu \left(1 + \frac{A}{\sqrt{AA'}}\right), \quad A = D_0 - \mu. \]  
(The allowed range of $\mu > 0$ will be commented on below). If we start from the Wilson fermion, $D_0 = D_W$, we arrive at the Neuberger fermion \cite{7}.

However, here we are interested in improvements in various respects due to a better choice of $D_0$ \cite{8}.

Our guide-line for the search of a better $D_0$ is the following observation: if $D_0$ is a GW operator already (for some fixed GW kernel $R$), then it coincides with the resulting overlap operator, $D_{\text{ov}} = D_0$. In real life we are now going to construct an approximate GW operator within a short range, and we use it as $D_0$. Hence the notorious square root in eq. (3) is approximately constant, $\sqrt{AA'} \approx \mu$, and therefore
\[ D_{\text{ov}} \approx D_0. \]  

For the free fermion, the perfect action can be constructed and parametrised explicitly \cite{9}, though it involves an infinite number of couplings. Still this fermion formulation is local, because the absolute value of these couplings decays exponentially with the distance between $\bar{\psi} \text{ and } \psi$.

We construct $D_0$ from the couplings of a truncated perfect free fermion. The truncation is done so that only couplings inside a unit hypercube survive, hence we arrive at a hypercube fermion (HF). Then we gauge this HF (we distribute the coupling over the link paths) by using just very few parameters, in such a way that the violation of the GWR is minimised. The criterion for this violation is proximity of the fermion spectrum to the unit GW circle, which corresponds to $\mu = 1$.

Even if we only perform “minimal gauging” (shortest lattice paths only, see below), the re-
resulting operator $D_{HF}$ is promising for scaling and it is almost rotationally invariant [10] — due to the perfect action background — although it is short-ranged.

If we now insert $D_0 = D_{HF}$ in the overlap formula, we expect a number of virtues for $D_{ov}$, which are all based on relation (4):

- $D_{ov}$ is promising for a good scaling behaviour and approximate rotational invariance, properties which are inherited from $D_0$.

- We expect $D_{ov}$ to have a high level of locality (a fast exponential decay of the correlations), since $D_0$ is ultralocal and long-range couplings can be turned on just slightly by the overlap formula.

- The iterative transition from $D_0$ to $D_{ov}$ is fast, since we already start off in the right vicinity.

This is in contrast to the Neuberger fermion, which does a rather poor job with respect to all these properties. The above predictions have been tested and confirmed in a comprehensive study of the 2-flavour Schwinger model [11]. We used a 2d HF, which had (amazingly) a similar scaling quality as the very mildly truncated, classically perfect fermion of Ref. [4]. The superiority of the resulting $D_{ov}$ (improved overlap fermion) over the Neuberger fermion (or standard overlap fermion) was striking in all the respects listed above.

We are now carrying on this program to (quenched) QCD [13]. Locality properties of free 4d improved overlap fermions have already been discussed in Ref. [8], and first results for QCD have been reported in Ref. [12]. The same concept has also been adopted in Ref. [14], which presents some results with respect to the last property (speed of the transition), based on a very simple choice of $D_0$. On the other hand, sophisticated and complicated approximate GW fermions have been constructed in Ref. [15].

Following the same lines, one may also work on improved domain wall fermions by optimising the choice of the 4d operator that corresponds to $D_0$ [8]. Recent proposals focus on accelerating the transition to exact chirality, which is expressed here in terms of the required extent of the extra dimension [10].

2. Construction of $D_0$

We now describe explicitly the construction of our HF, which approximates a GW fermion, and which is also promising in other respects. We proceed gradually in a sequence of steps.

2.1. Truncated perfect free fermion

As we mentioned earlier, perfect actions for free fermions can be constructed analytically, where the term $R$ occurs in the renormalisation group transformation term. The locality is optimal for $R_{x,y} = \delta_{x,y}$ (i.e. $\mu = 1$) [9], which is the standard GW kernel, and which we are going to use in the following.

We write the Dirac operator of the free perfect fermion as

$$D(x - y) = \rho(x - y)\gamma_{\mu} + \lambda(x - y),$$

where we denote $\rho, \lambda$ as the vector term and the scalar term, respectively. We truncate both terms by imposing periodic boundary conditions, so that we arrive at a free HF. The explicit couplings inside a unit hypercube are given in Ref. [10], Table 1. The scaling of this free HF is excellent [10], and its spectrum is very close to a GW unit circle [8], hence it is a good approximation to a GW fermion.

The resulting free overlap HF has the expected virtues, in particular good scaling and locality [8].

2.2. Minimal gauging

We now proceed to quenched QCD, and we always use the plaquette gauge action. Tests with improved gauge actions are on the way.

Our point of departure is a minimal gauging of the HF: the free couplings are attached to the shortest lattice paths only, in equal parts where several shortest paths coexist. This is the simplest version of a HF in gauge theory, but the harmony of the truncated free couplings leads to a beautiful pion dispersion relation, even at strong coupling, see Ref. [10], Fig. 10. On the other hand, this kind of gauging implies a strong

\[2^{They seem to be indeed useful for chirality, see last reference in [13].]
mass renormalisation — comparable to the Wilson fermion. The reason is that all paths are suppressed by the gauge field (compared to the free case), whereas the coupling between \( \bar{\psi} \) and \( \psi \) on the same site is unaltered. For instance, at \( \beta = 5 \) we obtain a “pion mass” of 3.0 \([10]\).

This effect is also visible from the fermionic spectrum: again at \( \beta = 5 \) the right arc still follows closely the GW circle — unlike the Wilson fermion spectrum, which extends to large real parts. However, the physically crucial left arc is absent in both cases, see Fig. 1.

\[ \begin{array}{c}
\text{\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure1.png}
\caption{The fermionic spectrum for the minimally gauged HF and for the Wilson fermion, in a typical configuration at \( \beta = 5 \).}
\end{figure}}
\end{array} \]

In such a situation, the overlap formula — which is supposed to provide a projection of the spectrum onto a GW circle — is not applicable any more: there is no suitable value of \( \mu \), which is the centre of the circle to be mapped on. Wherever we choose it, we would be confronted frequently with too many mappings to the left (revival of the doubling problem) or to the right arc (mass renormalisation is back) or both.

Now it is of interest where the applicability of the overlap formula sets in. At \( \beta \approx 5.4 \) the coupling is still too strong, whereas at \( \beta \gtrsim 5.6 \) we are statistically on safe grounds for a simple operator \( D_0 \) \([12]\).

\[ \begin{array}{c}
\text{\begin{figure}
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\includegraphics[width=\textwidth]{figure2.png}
\caption{HF spectra at \( \beta = 6 \) on a \( 4^4 \) lattice at critical link amplification \( 1/u \) without fat links (\( \alpha = 0 \)) and with fat links (\( \alpha = 0.3 \)).}
\end{figure}}
\end{array} \]

So far, we show the full fermionic spectra on small \( 4^4 \) lattices. From our experience, this is sufficient to obtain the qualitatively correct impression about the performance of a lattice Dirac operator. The fact that the arc close to zero tends to be absent is not due to the fermion formulation, but solely due to the small lattice. Later we will show this arc specifically also on \( 8^4 \) lattices, in order to provide a more complete picture.

2.3. Criticality through link amplification

We now go beyond minimal gauging by introducing a few extra parameters and optimising them so that the GWR violation is minimised at \( \beta = 6 \).

First we attach a amplification factor \( 1/u \) (\( u \lesssim 1 \)) to each link. The idea is to compensate the mean link suppression due to the gauge field. At \( \beta = 6 \) we obtain criticality at \( u \simeq 0.8 \). This already provides a decent approximation to a GW fermion, see Fig. 3.

\[ \begin{array}{c}
\text{\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure3.png}
\caption{HF spectra at \( \beta = 6 \) on a \( 4^4 \) lattice at critical link amplification \( 1/u \) without fat links (\( \alpha = 0 \)) and with fat links (\( \alpha = 0.3 \)).}
\end{figure}}
\end{array} \]

2.4. Fat links and vector term suppression

We now introduce fat links by globally substituting all links as

\[ \text{link} \rightarrow (1 - \alpha) \text{link} + \frac{\alpha}{6} \sum \text{staples}. \]

It turns out that for instance \( \alpha = 0.3 \) is a useful value: it helps to move the upper (resp. lower) arc charge by the index theorem. What we achieve at \( \beta \gtrsim 5.6 \) is that this transition is very quick, i.e. for most configurations occurring at that coupling strength, all (almost) real eigenvalues clearly belong to the left or the right arc.

\[ \begin{array}{c}
\text{\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure4.png}
\caption{HF spectra at \( \beta = 6 \) on a \( 4^4 \) lattice at critical link amplification \( 1/u \) without fat links (\( \alpha = 0 \)) and with fat links (\( \alpha = 0.3 \)).}
\end{figure}}
\end{array} \]
closer to the circle, and it also pulls the eigenvalues closer together, which are both desired effects, as illustrated in Fig. 2.

On the other hand, a sequence of experiments suggests that the *clover term* is not a very powerful tool to improve the GWR approximation. Hence we omit it, since we only want to include new ingredients if they really yield a significant progress.

An exception from that rule are the factors that we attach to the links, since they require practically no computational effort. Hence we can also introduce different link factors for the scalar term $\lambda$ and the vector term $\rho_\mu$. The former is responsible for the chiral limit, so we leave it unaltered at $u = 0.8$. However, we suppress the vector term a little, because it is responsible for the imaginary part of the fermionic spectra, which are a bit too large so far. So now we multiply in $\rho_\mu$ only the links by $v/u$, $v \lesssim 1$. By tuning the value of $v$ we can make the above spectra follow the shape of the GW circle. Still the fat link is useful to suppress the radial fluctuations of the eigenvalues. We use again $\alpha = 0.3$, and find the suitable vector link suppression to be $v = 0.92$. This leads to the quite satisfactory spectrum shown in Fig. 3.

3. Convergence to $D_{ov}$

In $d = 4$ the troublesome square root in the overlap formula (3) can only be approximated iteratively. A simple approach is the expansion of the inverse square root in a series in $A^\dagger A - \mu^2$. This converges for all eigenvalues only if we start from a good GW fermion approximation $D_0$, and then the convergence is fast, as we have shown in the Schwinger model [11].

We now turn our attention to the usual method which approximates the sign function $\epsilon$ in

$$D_{ov} = \mu[1 + \gamma_5 \epsilon(H)] , \quad H = \gamma_5 (D_0 - \mu) = H^\dagger \ (5)$$

by a polynomial in $H$.

The histograms for typical spectra of $H_W$ and $H_{HF}$ at $\beta = 6$ are shown in Fig. 3 (on top). For the HF (with $\alpha = 0.3$, $u = 0.76$, $v = 0.92$) the spectrum is already nicely peaked near $\pm 1$, whereas the Wilson fermion yields a broad distribution.

![Figure 3](image_url)

*Figure 3. The HF on a $4^4$ lattice with critical link amplification, fat links and a suppression of the vector term. We also show the “continuation” around 0 on a $8^4$ lattice with the same parameters, i.e. $u = 0.76$, $\alpha = 0.3$, $v = 0.92$."

In order to make the polynomial approximation applicable for all eigenvalues, we have to re-scale the spectra such that they are confined in the interval $[-1, 1]$, see Fig. 4 (below). This does not affect the spectrum of $H_{HF}$ too much, and in particular there is a large gap around 0, where any polynomial approximation of the sign function has its largest error. On the other hand, for
Figure 5. The spectra of approximate overlap fermions, where the sign function is replaced by a polynomial of degree 21. We use a configuration typical at $\beta = 6$ and start from $D_0 = D_W$ (stars) resp. from $D_0 = D_{HF}$ (crosses).

$H_W$ there is a significant eigenvalue density in the vicinity of 0, which shows again that here it is far more demanding to enforce convergence to a GW fermion.

We illustrate the difference by using a linear combination of Chebyshev polynomials (as suggested in Ref. [17]) with maximal degree 21 to approximate the sign function in the overlap formula (5). For a typical configurations at $\beta = 6$ (on a $4^4$ lattice) this leads to the spectra shown in Fig. 5 for the Wilson fermion resp. the HF. We see that the latter is clearly superior. This gain might already compensate the computational overhead by a factor of $O(10)$ in the application of $D_{HF}$.

4. Conclusions

A good approximation to a GW fermion in QCD at $\beta = 6$ has been constructed, using only 10 independent parameters. This HF is ready to be inserted in the overlap formula (3). This works down to $\beta \approx 5.6$, and it leads to an exact GW fermion. There are good reasons to expect that the resulting GW fermion is superior over the standard Neuberger fermion with respect to scaling, rotational symmetry and locality. We tested the speed of convergence towards an overlap fermion if the sign function in the overlap formula is replaced by Chebyshev polynomials. Also with this respect we found a significant gain if we start from $D_{HF}$ instead of $D_W$. This effect will be discussed in detail in Ref. [13].

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