Overlap Hypercube Fermions in QCD

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We present simulation results obtained with overlap hypercube fermions in QCD near the chiral limit. We relate our results to chiral perturbation theory in both, the $\epsilon$-regime and in the $p$-regime. In particular we measured the pion decay constant by different methods, as well as the chiral condensate, light meson masses, the PCAC quark mass and the renormalisation constant $Z_A$.

1. INTRODUCTION

We report on our recent simulation results for QCD on the lattice with chirally symmetric fermions. The aim is to relate our numerical results to chiral perturbation theory ($\chi$PT), as an effective theory of the strong interaction at low energies. The simulation of QCD, as the fundamental theory, allows for a determination of free parameters in this effective theory.

In Section 2 we review the construction of the hypercube fermion (HF) and show recent applications at finite temperature. We then proceed to the corresponding overlap hypercube operator, and we present results on its locality at strong gauge coupling.

In Section 3 we turn our interest to the $\epsilon$-regime, which is the main focus of this work. In this setting, the linear size of the volume is shorter than the correlation length (which is given by the inverse pion mass). As an important virtue, evaluations in this regime do not need an extrapolation to the infinite volume: physical quantities — in particular the Low Energy Constants (LEC) of the chiral Lagrangian — can be identified directly in a small box, with their values in infinite volume.

In Section 4 we add results obtained in the (standard) $p$-regime, where the $\chi$PT works by expanding in the momenta of the light mesons involved, and in Section 5 we arrive at our conclusions.

Throughout this work we refer to quenched simulations using the (standard) Wilson gauge action, and we deal with a physical volume of $V = (1.48 \text{ fm})^3 \times 2.96 \text{ fm}$ at two lattice spacings $a$ (measured by the Sommer scale $\Lambda$). Preliminary results were presented before in Refs. [2].

2. OVERLAP HYPERCUBE FERMIONS

For free fermions, perfect lattice actions are known analytically [3]. The corresponding lattice Dirac operator can be written as

$$D_{x,y} = \gamma_\mu \rho_\mu (x-y) + \lambda (x-y),$$

(1)

with closed expression for $\rho_* \text{ and } \lambda \text{ in momentum space}$. Such actions emerge from iterated renormalisation group transformations, hence they are free of any lattice artifacts regarding scaling and chirality. $D_{x,y}$ is local (for non-vanishing $\lambda$) but its range is infinite. Hence we tuned the renormalisation group parameters for an optimal locality of $D_{x,y}$; then we truncate it by means of periodic boundary conditions so that the supports of $\rho_\mu (x-y) \text{ and } \lambda (x-y)$ are contained in $\{|x_\nu - y_\nu| \leq 1\}$ for $\nu = 1 \ldots 4 \text{ (in lattice units, } a = 1)$. This truncation yields the free Hypercube Fermion (HF) which still has excellent scaling and chirality properties [4].

The HF is gauged by (normalised) sums over the shortest lattice paths between its sites. The paths correspond to products of fat link gauge variables, which are simply built as $U_\mu (x) \rightarrow (1-\alpha) U_\mu (x) + \frac{\alpha}{a} \sum \text{ staples}$. Finally the links are...
amplified to restore criticality and to minimise the violation of the Ginsparg-Wilson relation.

Due to the truncation and the imperfect gauging procedure, the scaling and chirality are somewhat distorted. Still the HF has highly favourable features, particularly in thermodynamics [4,5]. As an example, we show in Fig. 1 recent results for the spectral function $\sigma_{PS}$, which reveal a continuum-like behaviour up to much larger energies than it emerges for the Wilson fermion.

Figure 1. The spectral function $\sigma_{PS}$, as a function of the Matsubara frequencies $\omega$, at $T_c = \infty$ (on top, free case) and at finite $T_c$ (below, interacting case) [5]. These results are obtained from lattice data using the Maximum Entropy Method, as suggested in Ref. [6].

Exact chirality can be recovered by inserting the HF into the overlap formula [7]

$$D_{ov}^{(0)} = \rho(1 + A/\sqrt{A^\dagger A}), \quad A := D_0 - \rho,$$

where $\rho \geq 1$ and $D_0$ is some lattice Dirac operator, with $D_0 = \gamma_5 D_0^\dagger \gamma_5$ (\gamma_5\text{-Hermiticity}).

- The standard formulation [8] inserts the Wilson Dirac operator, $D_0 = D_W$, which is then drastically changed in eq. (2). We denote the resulting standard overlap operator, or Neuberger operator, as $D_{ov-W}$.
- Here we mainly study the case where instead the HF is inserted in the overlap formula (2), $D_0 = D_{HF}$ [9]. This yields the operator $D_{ov-HF}$, which describes the overlap-HF.

In both cases one arrives at exact solutions to the Ginsparg-Wilson relation [10], and therefore at an exact, lattice modified chiral symmetry [11]. However, in contrast to $D_W$, $D_{HF}$ is approximately chiral already, hence its transformation by the overlap formula (2), $D_{HF} \rightarrow D_{ov-HF}$, is only a modest modification. Therefore, the virtues of the HF are essentially inherited by the overlap-HF. Compared to $D_{ov-W}$, the degrees of locality and of approximate rotation symmetry are highly improved [9,11,15,16]. If the gauge coupling is not too strong, the maximal impact of a unit source on a sink, as well as the maximal violation of rotation symmetry, decay exponentially in the distance. For instance, at $\beta = 6$ the exponent of these decays is almost doubled for the overlap-HF compared to $D_{ov-W}$ [15]. (In the latter case, locality was first studied in Ref. [17].)

Here we are going to show mostly results at $\beta = 5.85$, which corresponds to a lattice spacing of $a \approx 0.123$ fm. We build the fat link with $\alpha = 0.52$ and amplify all link variables by a factor $u = 1.28$ (in the vector term we multiply another factor of 0.96). This is similar (but not exactly equivalent) to choosing the parameter $\rho$ in $D_{ov-W}$; for $D_{ov-HF}$ we fix $\rho = 1$. These parameters are chosen as a compromise between optimising the locality and the condition number of $A^\dagger A$. Fig. 2 (on top) shows that the locality is significantly improved upon $D_{ov-W}$ (at $\rho = 1.6$) [16].

In Fig. 2 (below) we illustrate the locality at strong gauge coupling: at $\beta = 5.7$ ($a \approx 0.17$ fm)

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2 The correctness of the axial anomaly in all topological sectors has been verified for the standard overlap operator in Ref. [14], and for the overlap HF in Ref. [13].
3. EVALUATION OF THE LEADING LOW ENERGY CONSTANTS IN THE $\epsilon$-REGIME

In the $\epsilon$-regime [18] the correlation length exceeds the box length, $1/m_\pi > L$, and the observables strongly depend on the topological sector [19]. Squeezing pions into such a tiny box may not be a realistic situation. Still, there is a striking motivation for studying this regime: it allows for an evaluation of the LEC with their values in infinite volume, i.e. with their physical values. (Unfortunately, quenching brings in logarithmic finite size effects [20], but there is a window of volumes with decent values nevertheless).

We first take a look at the overlap-HF indices: for 1013 configurations we obtained the histogram in Fig. 3 (on top). Fig. 3 (below) shows our results for the topological susceptibility, compared to the continuum extrapolation of Ref. [21], which used $D_{\text{ov-W}}$. Our susceptibilities are somewhat larger, but a rough continuum extrapolation agrees well with Ref. [21].

3.1. Link to the chiral Random Matrix Theory

Chiral Random Matrix Theory (RMT) conjectures the densities $\rho_n^{(\nu)}(z)$ of the lowest Dirac eigenvalues $\lambda$ in the $\epsilon$-regime [22], where $z := \lambda \Sigma V$. $n = 1, 2, \ldots$ numerates the lowest non-zero eigenvalues and $\nu$ is the fermion index, which is identified with the topological charge [11]. This RMT conjecture holds to a good precision for the lowest $n$ and $|\nu|$, if $L$ exceeds some lower limit (about 1.1...1.5 fm, depending on the exact criterion) [23]. Then the fit determines the scalar condensate $\Sigma$. From the cumulative density of the first eigenvalue in the topologically neutral sector, the fit implies a chiral condensate of $\Sigma = (299(8) \text{ MeV})^3$ for the overlap HF, in good agreement with the result of $\Sigma = (300(7) \text{ MeV})^3$ for the standard overlap operator, see Fig. 4.

3.2. Zero-mode contributions to the pseudoscalar correlation

We stay in the chiral limit and evaluate the time derivative of the zero-mode contribution to the correlation of the pseudo-scalar density $P = \ldots$
The cumulative density of the first Dirac eigenvalue \( \lambda_1 \) in the sector \( \nu = 0 \) — stereographically projected and re-scaled with \( \Sigma V \) at optimal \( \Sigma \) — compared to the RMT prediction.

“Str” is the corresponding “supertrace”, and \( M \) is the diagonal matrix of fermion masses. The peculiarity of the quenched chiral Lagrangian is the presence of a scalar field \( \Phi \). \( \mathcal{L}^{\text{NNLO}} \) contains five quenched LEC: \( F_\pi, \Sigma, K, m_0 \) and \( \alpha_0 \).

We consider the first term in the Taylor expansion of \( C'_{[\nu]}(t) \) around \( T/2 \). In a box \( L^3 \times T \) it takes the form \[ C'_{[\nu]}(t) \approx \frac{D^{\text{NNLO}}_{[\nu]}(F_\pi, \langle \nu^2 \rangle, \alpha)}{T} + \mathcal{O} \left( \left( \frac{s}{T} \right)^3 \right), \] (4)

with \( s := t - T/2 \) and \( \alpha := \alpha_0 - 2N_cKF_\pi/\Sigma \). The dependence on \( \langle \nu^2 \rangle \) originates from the Witten-Veneziano formula \[ C'_{[\nu]}(t) \approx \frac{D^{\text{NNLO}}_{[\nu]}(F_\pi, \langle \nu^2 \rangle, \alpha)}{T} + \mathcal{O}(\epsilon). \]

We analysed the zero-modes that we collected at \( \beta = 5.85 \) on a \( 12^3 \times 24 \) lattice, and at \( \beta = 6 \) on \( 16^3 \times 32 \). In both cases, the physical volume amounts again to \( (1.48 \text{ fm})^3 \times 2.96 \text{ fm} \). This is expected to be sufficiently large, referring to our experience with the chiral Random Matrix Theory \[ \mathcal{L}^{\text{NNLO}} \] and to the behaviour of the axial correlators in the \( \epsilon \)-regime (cf. Subsection 3.3). Our statistics is listed in Table \ref{tab:statistics}. We fixed the value of \( \langle \nu^2 \rangle \) from our simulations, since it can deviate significantly from the continuum extrapolation, as Fig. \ref{fig:overlap_density} (below) shows.

Then we performed a combined two parameter fit of the leading term in eq. (4) to our data in the

\[ C'_{[\nu]}(t) \approx \frac{D^{\text{NNLO}}_{[\nu]}(F_\pi, \langle \nu^2 \rangle, \alpha)}{T} + \mathcal{O}(\epsilon). \]
topological sectors $|\nu| = 1, 2$ over the intervals $s \in [-s_{\text{max}}, s_{\text{max}}]$, with $s_{\text{max}} = 1 \ldots 3$. Our results are shown in Fig. 5 and in Table 1. Our results for $F_\pi$ and $\alpha$ are a little lower than the results reported in Ref. [24] (for the Neuberger operator in isotropic boxes).

### Table 1

| $\rho$ | $(\nu^4)$ | $|\nu| = 1$ | $|\nu| = 2$ | $F_\pi$ [MeV] | $\alpha$ |
|--------|----------|-----------|-----------|-------------|--------|
| overlap-HF $12^4 \times 24$, $\beta = 5.85$ | 1 | 10.8 | 221 | 192 | 80 $\pm$ 14 | $-17 \pm 10$ |
| standard ov. $12^4 \times 24$, $\beta = 5.85$ | 1.6 | 11.5 | 232 | 180 | 74 $\pm$ 10 | $-19 \pm 8$ |
| standard ov. $16^3 \times 32$, $\beta = 6$ | 1.6 | 10.5 | 115 | 94 | 75 $\pm$ 24 | $-21 \pm 15$ |

Statistics and results for $F_\pi$ and $\alpha$, based on the zero-mode contributions to $\langle PP \rangle$. The values for $F_\pi$ and $\alpha$ in the last two columns correspond to the fitting range $s_{\text{max}} = 1$.

The Low Energy Constants $F_\pi$ and $\alpha$, determined from the zero-mode contributions to $\langle PP \rangle$, against the width of the fitting range $s_{\text{max}}$.

Figure 5. The Low Energy Constants $F_\pi$ and $\alpha$, determined from the zero-mode contributions to $\langle PP \rangle$, against the width of the fitting range $s_{\text{max}}$.

However, we see that our values of $F_\pi$ and $\alpha$ agree well for different overlap fermions and for two lattice spacings. This result for $F_\pi$ is close to the physical value — extrapolated to the chiral limit — of 86 MeV [28], but below typical quenched values, see Subsection 3.3.

### 3.3. Axial vector correlations

In quenched chPT, the axial vector correlator depends to leading order only on the LEC $\Sigma$ and $F_\pi$ [27]. The prediction for $\langle A_4(t)A_4(0) \rangle$ (with $A_4(t) := \sum x_\psi(x,t)\gamma_5\gamma_\mu\psi(x,t)$, i.e. the bare axial current at $\vec{p} = 0$) is a parabola with a minimum at $t = T/2$, where $F_\pi^2/T$ enters as an additive constant. In a previous study we observed that $L$ should again be above 1 fm for this prediction to work, and that the history in the sector $\nu = 0$ may be plagued by spikes, related to the occurrence of very small non-zero eigenvalues [28]. (This leads to the requirement of a large statistics, but a method called Low Mode Averaging was then invented as an attempt to overcome this problem [29].) In the non-trivial sectors, $\Sigma$ can hardly be determined, but $F_\pi$ can be evaluated [28, 30]. Fig. 6 shows our current results with three (bare) quark masses $m_q$ in the $\epsilon$-regime, in the sector $|\nu| = 1$ and 2. The (flavour degenerated) mass is incorporated in the overlap operator as

$$D_{ov}(m_q) = \left(1 - \frac{m_q}{2\rho}\right)D_{ov}^{(0)} + m_q.$$ (5)

Our result is based on 45 propagators for each mass in the sector $|\nu| = 1$, and 10 propagators for each mass in the sector $|\nu| = 2$. Inserting the RMT result of $\Sigma \simeq (299 \text{ MeV})^3$, as well as the renormalisation constant $Z_A = 1.17$ (see Section 4), a global fit leads to $F_\pi = (113 \pm 7) \text{ MeV}$, in agreement with other quenched results [20, 24, 30].

### 4. RESULTS IN THE $p$-REGIME

At last we present our results in the $p$-regime, which is characterised by a box length...
The subtraction of the scalar density is useful and follows well the expected behaviour of quenched $\chi$PT. (Our quark masses correspond to $\Sigma m_q = 0.83, 2.5$ and 4.2.)

$L \gg 1/m_\pi$, so that the $p$-expansion of $\chi$PT \cite{Fettes:2008} applies. We consider once more $\beta = 5.85$, a lattice of size $12^3 \times 24$ and the bare quark masses $am_q = 0.01, 0.02, 0.04, 0.06, 0.08$ and 0.1 (in physical units: $m_q = 16.1$ MeV...161 MeV).

We computed 100 overlap-HF propagators, and we first evaluated $m_\pi$ in three different ways:

1. From the pseudoscalar correlator $\langle P(t)P(0) \rangle$.
2. From the axial vector correlator $\langle A_4(t)A_4(0) \rangle$.
3. From $\langle P(t)P(0) - S(t)S(0) \rangle$, where $S = \psi\bar{\psi}$. The subtraction of the scalar density is useful at small $m_q$ to avoid the contamination by zero modes.

The results are shown in Fig. 6 (on top): they follow well the expected behaviour $am_\pi^2 \propto m_q$, in particular for $(PP-SS)$. Our smallest pion mass in this plot, $m_\pi \simeq 289$ MeV, has Compton wave length $\approx L/2$, hence this point is at the edge of the $p$-regime.

Fig. 6 (below) shows the corresponding results for the vector meson mass, with a (linear) chiral extrapolation to $m_\rho = 1017(39)$ MeV. Generally, quenched results tend to be above the physical $\rho$-mass. Our result is in agreement with a similar study using $D_{ov-W}$ \cite{M"uller:2006}, but somewhat above the (quenched) world data for $m_\rho$ \cite{Pelaez:2004}, (which are mostly obtained with chiral symmetry breaking lattice fermions).

![Figure 6](image1.png)

**Figure 6.** Results for the axial vector correlator at $am_q = 0.001, 0.003$ and 0.005 in the sectors $|\nu| = 1$ (red, larger around the centre) and 2 (blue), and fits to the formulae of quenched $\chi$PT. (Our quark masses correspond to $\Sigma m_q = 0.83, 2.5$ and 4.2.)

In Fig. 7 (on top) we show the PCAC quark mass obtained from the axial Ward identity,

$$m_{PCAC} = \frac{\sum_x \langle \partial_t A_4^\dagger(x) P(0) \rangle}{2 | \sum_x \langle P^\dagger(x) P(0) \rangle |}.$$ \hspace{1cm} (6)

We observe also here a behaviour which is nearly linear in $m_q$, with a chiral extrapolation to $am_{PCAC}(m_q = 0) = -0.00029(64)$.

Remarkably, $m_{PCAC}$ is close to $m_q$, which is not the case for $D_{ov-W}$ \cite{M"uller:2006}. Consequently the renormalisation constant $Z_A = m_q/m_{PCAC}$ is close to 1; it has the chiral extrapolation $Z_A = 1.17(2)$, which has been used already in Subsection 3.3. This is in contrast to the large $Z_A$ factors obtained for $D_{ov-W}$: at $\beta = 5.85$ ($\rho = 1.6$), $Z_A \simeq 1.45$ was measured \cite{M"uller:2006}, and at $\beta = 6$ ($\rho = 1.4$) even $Z_A \simeq 1.55$ \cite{M"uller:2006}.

Finally we reconsider the pion decay constant,
Figure 8. The PCAC quark mass of eq. (6), and the renormalisation constant $Z_A = m_q/m_{PCAC}$, now evaluated in the direct way, according to

$$F_\pi = \frac{2m_q}{m_\pi^2} \langle 0|P|\pi \rangle ,$$

(7)

by using either $PP$ or $PP - SS$, see Fig. 9. The linear extrapolation to $m_q = 0$ yields $F_{\pi, PP} = 111.5(2.5)$ MeV, resp. $F_{\pi, PP - SS} = 104(9)$ MeV, which is compatible with the result in Subsection 3.2. In particular the behaviour of the $(PP - SS)$ result for $F_\pi$ at small $m_q$ calls for an evaluation at yet smaller quark masses, which was reported in Section 3.

5. CONCLUSIONS

The HF operator is approximately chiral and it has favourable properties in particular in thermodynamics. It can be inserted into the overlap formula, which yields the overlap-HF. This is a formulation of chiral lattice fermions with better rotation symmetry and locality than the standard formulation. Therefore it provides access to chiral fermions on coarser lattices.

In the $\epsilon$-regime we evaluated — at tiny quark masses — the pion decay constant from the axial vector correlator. Directly in the chiral limit we obtained results for the chiral condensate from the Dirac spectrum. Moreover, from the zero-mode contribution to the pseudoscalar correlator, we found again values of $F_\pi$ and the parameter $\alpha$ (a quenching specific LEC). The results are very similar for two lattice spacings and different overlap operators. Our result for $F_\pi$ obtained with this method (in the given volume) is close to the physical value (in the chiral limit), but below other quenched values.\(^3\)

We add that a topology conserving gauge action could be helpful in that regime.\(^3\)

In the $p$-regime we obtained results for $m_\pi$, $m_\rho$ and $F_\pi$. Compared to the standard overlap fermion, $m_{PCAC}$ is closer to the bare quark mass $m_q$, hence $Z_A$ is much closer to 1, which is pleasant for a connection to perturbation theory. Here we measured $F_\pi$ directly, and the chiral extrapolation of this result agrees (within the errors) with the value obtained in the $\epsilon$-regime from the axial vector correlator.

\(^3\)The two methods applied for the axial vector and the pseudoscalar correlator differ by a subtlety in the quenched counting rules for the $\epsilon$-expansion.
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