## Overlap Hypercube Fermions

## in QCD with Light Quarks

I. Construction of the overlap HF

Locality, rotation symmetry and condition number
II. Applications in the $p$-regime :
$m_{q}$ vs. $m_{\pi}, m_{\rho}, m_{\mathrm{PCAC}}, Z_{A}$ and $F_{\pi}$
III. Applications in the $\epsilon$-regime : $F_{\pi}$ and $\Sigma$

Topological charges and susceptibility
Zero-mode contributions to $\langle P P\rangle$ in $\chi$ limit
W. Bietenholz (HU Berlin) and S. Shcheredin (Bielefeld), $\chi L F$

## I. Construction of the Overlap HF

For free fermions, the perfect lattice action is known analytically (W.B./Wiese '95). Dirac operator:

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

with closed expressions for $\rho_{\mu}(p), \lambda(p)$.
Based on iterated RG transformations $\rightarrow$ no lattice artifacts
Range of $D_{x, y}$ is infinite $\rightarrow$ optimise the RGT for locality, then truncate by periodic b.c. to a $3^{4}$ hypercube $\rightarrow \operatorname{supp}\left[\rho_{\mu}(x-y), \lambda(x-y)\right] \subset\left\{\left|x_{\nu}-y_{\nu}\right| \leq 1\right\}, \nu=1 \ldots 4$
"Hypercube Fermion" (HF), still excellent scaling (W.B./Brower/Chandrasekharan/Wiese, '96).

Gauging: sum over shortest lattice paths, plus fat links $U_{\mu}(x) \rightarrow(1-\alpha) U_{\mu}(x)+\frac{\alpha}{6} \sum$ staples ; link amplification $\rightarrow$ criticality

Truncation and imperfect gauging $\rightarrow$ scaling and chirality somewhat distorted. Chirality can be corrected again by inserting the HF into the overlap formula (H. Neuberger, '97) :

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

where $D_{0}$ is some lattice Dirac operator (with $D_{0}=\gamma_{5} D_{0}^{\dagger} \gamma_{5}$ ).

- Standard overlap fermion: based on $D_{0}=D_{\text {Wilson }}$

Drastic change : $D_{\text {Wilson }} \rightarrow D_{\text {ov-W }}$

- Overlap HF: $D_{0}=D_{\mathrm{HF}}$
$D_{\mathrm{HF}}$ is approx. chiral already $\rightarrow$ modest modification : $D_{\mathrm{HF}} \rightarrow D_{\mathrm{ov}-\mathrm{HF}}$
Both are Ginsparg-Wilson operators $\rightarrow$ exact $\chi$ sym. (P. Hasenfratz, '98, M. Lüscher, '98)
$\Rightarrow$ Virtues of the HF are essentially inherited by $D_{\text {ov-HF }}$ : high degree of locality, approx. rotation symmetry, fast convergence
Examples at $\beta=6, V=12^{4}$, Wilson gauge action, quenched:




Overlap HF vs. standard overlap at $\rho=1.4$

- $f_{\max }(r)$ "maximal correlation" between unit source $\bar{\psi}_{x}$ and $\psi_{y}$ with $r=\|x-y\|_{1}$ (Hernández et al. '99)
- Measure for violation of rot. sym. : $f_{\max }(|x-y|)-f_{\min }(|x-y|)$
- Condition numbers $c_{k}$ :
(largest EV of $A^{\dagger} A$ ) / (smallest EV , after projecting out $k-1$ modes)
Gain factor $\approx 25 \rightarrow$ factor 5 in polynomial degree, vs. factor 15 of HF overhead


## Locality at strong coupling:



- $\beta=5.7 \quad(a \simeq 0.17 \mathrm{fm}): D_{\mathrm{ov}-\mathrm{W}}$ with optimal $\rho$ barely local $\overline{D_{\text {ov-HF }}}$ with optimal link amplification has powerful locality, stronger than $D_{\text {ov-W }}$ at $\beta=6, \rho=1.4$
- $\beta=5.6$ : for $D_{\text {ov-W }}$ locality collapses, no valid Dirac operator but $\mathbf{D}_{\text {ov-HF }}$ is still local

The overlap-HF formulation provides chiral fermions on coarser lattices.

## II. Applications in the $p$-Regime

$p$-regime : $p$ expansion of $\chi \mathrm{PT}$ is applicable, box length $\quad \mathrm{L} \gg \frac{1}{\mathrm{~m}_{\pi}}$
We consider $\beta=5.85 \quad(a \simeq 0.123 \mathrm{fm})$
$V=12^{3} \times 24, \quad V_{\text {phys }}=(1.48 \mathrm{fm})^{3} \times 2.96 \mathrm{fm}$
Bare quark masses : $a m_{q}=0.01,0.02,0.04,0.06,0.08,0.1$
$\triangleq \mathbf{m}_{\mathrm{q}} \simeq 16.1 \mathrm{MeV} \ldots 161 \mathrm{MeV}, \quad D_{\mathrm{ov}}\left(m_{q}\right)=\left(1-\frac{m_{q}}{2 \rho}\right) D_{\mathrm{ov}}^{(0)}+m_{q}$
$\left\{\right.$ At smallest $m_{q}$ close to $\epsilon$-regime \}
Statistics: 100 propagators
We evaluate the pion mass in three ways:

- Pseudoscalar correlator $\langle P P\rangle, \quad P=\bar{\psi} \gamma_{5} \psi$
- $\left\langle A_{4} A_{4}\right\rangle, \quad A_{4}=\bar{\psi} \gamma_{5} \gamma_{4} \psi$
- $\langle P P-S S\rangle, \quad S=\bar{\psi} \psi$ : subtraction useful at small $m_{q}$, avoids contamination by zero modes, which plagues quenched results

Pion mass

$m_{\pi}^{2} \propto m_{q} ;$ Intercept for $m_{\pi, P P-S S}^{2}\left(m_{q}=0\right)=-0.001(15)$
Hierarchy at small $m_{q}: m_{\pi, P P}>m_{\pi, A A}>m_{\pi, P P-S S}$
(agrees with P. Hasenfratz et al. '02)
Smallest pion mass : $m_{\pi, P P-S S}\left(a m_{q}=0.01\right) \simeq(279 \pm 32) \mathrm{MeV}$
$\rightarrow \frac{L}{\xi} \approx 2$, edge of $p$-regime
$\rho$-meson mass and quark mass according to the axial Ward identity:



Chiral extrapolation :

$$
\begin{aligned}
m_{\rho} & \in[978 \mathrm{MeV}, 1057 \mathrm{MeV}] \quad, \quad m_{\mathrm{PCAC}} \in[-0.00094,0.00035] \\
m_{\mathrm{PCAC}} & =\sum_{\vec{x}}\left\langle\partial_{4} A_{4}^{\dagger}(x) P(0)\right\rangle / 2 \sum_{\vec{x}}\left\langle P^{\dagger}(x) P(0)\right\rangle \quad\left(\text { for } D_{\mathrm{ov}-\mathrm{W}}, \text { see } \chi \mathrm{LF},{ }^{\prime} 04\right)
\end{aligned}
$$

This yields the renormalisation constant

$$
Z_{A}=\frac{m_{q}}{m_{\mathrm{PCAC}}}
$$

and the pion decay constant $\left.\quad F_{\pi}=\frac{2 m_{q}}{m_{\pi}^{2}}|\langle 0| P| \pi\right\rangle \mid$



Chiral extrapolation :

- $Z_{A}=1.17(2)$; much closer to 1 than $Z_{A}$ for standard overlap at same $\beta$
( $Z_{A} \simeq 1.45$ at $\rho=1.6, \chi$ LF ' $04 ; Z_{A} \simeq 1.55$ at $\beta=6, \rho=1.4$, Berruto et al. '03)
- $F_{\pi, P P} \in[109 \mathrm{MeV}, 114 \mathrm{MeV}], \quad F_{\pi, P P-S S} \in[95 \mathrm{MeV}, 113 \mathrm{MeV}]$
above theor. value in the $\chi$ limit: 86 MeV (Colangelo/Dürr, '04)
$\rightarrow$ to be reconsidered in the $\epsilon$-regime at smaller $m_{q} \ldots$


## III. Applications in the $\epsilon$-Regime

$\epsilon$-regime : $\frac{1}{m_{\pi}}>L$
In $\chi$ PT $p$-expansion fails due to dominant 0 -modes
But: analytical treatment of zero modes with collective variables (Gasser/Leutwyler, '87), higher modes captured by $\epsilon$-expansion

Motivation: unphysical setting, but physical values of the Low Energy Constants (LEC, free parameters in $\chi \mathbf{P T}, F_{\pi}, \Sigma \ldots$ ) can be evaluated in small volumes
$\rightarrow$ LEC at $V=\infty$.
Challenge for simulations with Ginsparg-Wilson fermions.
However: quenching $\rightarrow$ log. finite size effects (Damgaard, '01)
Peculiarity of $\epsilon$-regime: observables depend strongly on the topological sector (Leutwyler/Smilga, '92)

## Evaluation of $\Sigma$ from the Dirac Spectrum

$\chi$ Random Matrix Theory conjectures the densities of the low lying Dirac eigenvalues $\lambda$ in the $\epsilon$-regime (Damgaard/Nishigaki, '98) :

$$
\rho_{\mathbf{n}}^{(\nu)}(\mathbf{z})
$$

$z:=\lambda \Sigma V \quad$ (dim'less)
$n=1,2,3 \ldots$ (lowest eigenvalues, excluding zeros)
$\nu:=$ index $\equiv$ top. charge
W.B./Jansen/Shcheredin, Giusti/Lüscher/Weisz/Wittig, Galletly et al., '03 : $\chi$ RMT predictions hold for leading EVs if the volume is not too small ( $L \gtrsim 1.1 \mathrm{fm}$ )

Scalar condensate $\Sigma$ : only free parameter, determined by the fit.

$$
V=(1.48 \mathrm{fm})^{3} \times 2.96 \mathrm{fm} \text { at } a \simeq 0.12 \mathrm{fm}(\beta=5.85), \text { and } a \simeq 0.093 \mathrm{fm}(\beta=6)
$$



Prediction works well in particular for $|\nu|=0,1,2$
For the overlap-HF the fits yields : $\Sigma=(268(2) \mathrm{MeV})^{3}$

## Preliminary result for $F_{\pi}$ from the axial-vector correlator

Correlators to first order in quenched $\chi$ PT (q $\chi$ PT) (Damgaard et al., '02, '03)
$\langle$ Vector - Vector $\rangle=0 \quad$ (all orders)
$\langle S c a l a r-S c a l a r\rangle$ and $\langle P s e u d o s c a l a r-P s e u d o s c a l a r\rangle$ involve additional LEC, specific to quenching.
$\Rightarrow$ Focus on $\langle$ Axialvector - Axialvector $\rangle$
in leading order only $\Sigma$ and $F_{\pi}$
Bare axial current at $\vec{p}=\overrightarrow{0}: A_{\mu}(t)=\sum_{\vec{x}} \bar{\Psi}(t, \vec{x}) \gamma_{5} \gamma_{\mu} \Psi(t, \vec{x})$ $\left\langle A_{4}(t) A_{4}(0)\right\rangle$ in a volume $L^{3} \times T$ :


Parabola: min. at $t=T / 2 ; F_{\pi}^{2} / T$ : additive, $\Sigma \rightarrow$ curvature
W.B./Chiarappa/Jansen/Nagai/Shcheredin, '03 :

Simulations at $m_{q}=21.3 \mathrm{MeV}, \beta=6$ on $V=10^{3} \times 24$ and $12^{4}$

- First lattice failed; consistent with $\chi$ RMT study: $\mathrm{L} \simeq 0.98 \mathrm{fm}$ is too small
- MC history in $\nu=0$ has strong spikes, smoother at $\nu \neq 0$, Spikes exactly for conf's with very small EV, most frequent at $\nu=0$
\{ Remedy: "Low Mode Averaging", Giusti et al. '04 \}
Decent agreement with $\mathrm{q} \chi$ PT in $V=(1.12 \mathrm{fm})^{4},|\nu|=1$ : $F_{\pi}=(86.7 \pm 4.0) \mathrm{MeV}$

Renormalisation with $Z_{A} \simeq 1.55 \rightarrow F_{\pi}^{\mathrm{r}} \approx 130 \mathrm{MeV}>93 \mathrm{MeV}$.
$\Sigma$ cannot be extracted (curves hardly sensitive to $\Sigma=0$ or $\left.\Sigma=(250 \mathrm{MeV})^{3}\right)$.
\{ See also: Fukaya/Hashimoto/Ogawa, '05 \}

Preliminary result for overlap-HF $\left(12^{3} \times 24, \beta=5.85\right) 10$ propagators in each of the sectors $|\nu|=1,|\nu|=2 ; \quad m_{q}=1.6 \mathrm{MeV}, 4.8 \mathrm{MeV}, 8 \mathrm{MeV}$


Global fit with $\Sigma=(268 \mathrm{MeV})^{3}: F_{\pi}=(96 \pm 10) \mathrm{MeV}$
Renormalised: $F_{\pi}^{\mathrm{r}}=(104 \pm 9) \mathrm{MeV}$ (agrees with quenched literature)
Alternative method based on 0 -mode contributions to meson correlators in the $\chi$ limit: see below.

## Topological Charges :




Left: part of index histories for standard overlap and overlap-HF, same conf's, $\langle | \nu_{\mathrm{ov}-\mathrm{W}}-\nu_{\mathrm{ov}-\mathrm{HF}}| \rangle \approx 0.8$, max. deviation: 5

Right: charge histogram for overlap-HF, compatible with a Gaussian, parity (?)
(c.f. Alles/D'Elia/DiGiacomo, '05)

Topological susceptibility $\quad \chi=\frac{1}{\mathrm{~V}}\left\langle\nu^{2}\right\rangle \quad$ (relevant for mass of $\eta^{\prime}$ )


Comparison to the continuum limit by Del Debbio/Giusti/Pica '04 (for $\left\langle\nu^{2}\right\rangle r_{0}^{4} / V$ ).
Considering finite $a$ and $\rho=1.6$ : agreement within the errors
Overlap HF data closer to cont. limit (same confs at $\beta=5.85$ )

Giusti/Hernández/Laine/Weisz/Wittig '04: $\mathrm{q} \chi$ PT predictions for the

## ZERO-MODE CONTRIBUTIONS to $\langle P P\rangle_{|\nu|}$

$\Rightarrow$ from the zero-modes alone we can evaluate $F_{\pi}$ and $\alpha$
$\alpha$ : Low Energy Constant, specific to quenching, enters leading order of $\langle P P\rangle$.
$\mathcal{L}_{\mathrm{q} \chi \mathrm{PT}}^{(2)}$ is formulated with aux. scalar $\phi_{0}$, which supplements the quenching effect
$K$ : couples $\phi_{0} U$, plus $\quad \frac{1}{2} \alpha_{0}\left(\partial_{\mu} \phi_{0}\right)^{2}+\frac{1}{2} m_{0}^{2} \phi_{0}^{2}$
Count $m_{0}=\mathcal{O}(\epsilon)$ and define $\alpha=\alpha_{0}-4 N_{c}^{2} K F_{\pi} / \Sigma$
$\Rightarrow$ first order observables only involve $F_{\pi}$ and $\alpha$ (dim'less)
Pseudoscalar density $P=\bar{\psi} \gamma_{5} \psi$

$$
\begin{aligned}
\langle P(x) P(y)\rangle & =N_{f} P_{1}(x, y)-N_{f}^{2} P_{2}(x, y) \\
P_{1}(x, y) & =\operatorname{Tr}\left[i \gamma_{5}\left(D+m_{q}\right)^{-1}(x, y) \cdot i \gamma_{5}\left(D+m_{q}\right)^{-1}(y, x)\right] \\
P_{2}(x, y) & =\operatorname{Tr}\left[i \gamma_{5}\left(D+m_{q}\right)^{-1}(x, x)\right] \cdot \operatorname{Tr}\left[i \gamma_{5}\left(D+m_{q}\right)^{-1}(y, y)\right]
\end{aligned}
$$

Spectral decomposition of propagators $\rightarrow$ residuum given by zero modes:

$$
\begin{aligned}
\lim _{m_{q} \rightarrow 0}\left(m_{q} V\right)^{2}\langle P(x) P(0)\rangle_{\nu} & =N_{f} C_{|\nu|}^{(1)}(x)+N_{f}^{2} C_{|\nu|}^{(2)}(x) \\
\text { connected : } \quad C_{|\nu|}^{(1)}(x) & =-\left\langle v_{j}^{\dagger}(x) v_{k}(x) \cdot v_{k}^{\dagger}(0) v_{j}(0)\right\rangle_{\nu} \\
\text { disconnected : } \quad C_{|\nu|}^{(2)}(x) & =\left\langle v_{j}^{\dagger}(x) v_{j}(x) \cdot v_{k}^{\dagger}(0) v_{k}(0)\right\rangle_{\nu}
\end{aligned}
$$

summed over (exact) zero modes, $D v_{j}=0$.
Spatial average: $\frac{1}{V} \int d^{3} x P(x) P(0) \quad \rightarrow \quad C_{|\nu|}^{(i)}(t)$
Fits for $C_{|\nu|}^{(i)}(t)$ are troublesome; more handy:

$$
\left.\frac{1}{L^{2}} \frac{d}{d t} C_{|\nu|}^{(i)}(t)\right|_{t=T / 2}=D_{|\nu|}^{(i)} \cdot s+\mathcal{O}\left(s^{3}\right), \quad s=t-\frac{T}{2}
$$

Measure slopes $D_{|\nu|}^{(i)}$ up to $s= \pm 1, \pm 2, \ldots$, fits yield values for $\mathbf{F}_{\pi}, \alpha$

Combined fit for $F_{\pi}$ and $\alpha$ for zero-mode pseudoscalar correlators of standard overlap operator and the overlap-HF operator in $V=(1.48 \mathrm{fm})^{3} \times 2.96 \mathrm{fm}, \quad\left\langle\nu^{2}\right\rangle$ as measured in each case.

Statistics:

| Dirac operator | $\beta$ | lattice size |  | $\|\nu\|=\mathbf{1}$ | $\|\nu\|=\mathbf{2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| standard overlap | 5.85 | $12^{3} \times 24$ |  | $\mathbf{1 3 2}$ | $\mathbf{1 1 5}$ |
| overlap HF | 5.85 | $12^{3} \times 24$ |  | $\mathbf{2 2 1}$ | $\mathbf{1 9 2}$ |
| standard overlap | 6 | $16^{3} \times 32$ |  | $\mathbf{1 1 5}$ | $\mathbf{9 4}$ |


s: fitting range around $T / 2$.
In particular the overlap HF yields a neat plateau. $F_{\pi}=(80 \pm 14) \mathrm{MeV}, \alpha=-17 \pm 10$. Standard overlap data consistent. $F_{\pi}$ moves down compared to $\langle A A\rangle \quad$ (theory: 86 MeV at $m_{q}=0$ ).
Giusti et al. in $V \simeq(1.49 \mathrm{fm})^{4}: F_{\pi} \simeq(117 \pm 16) \mathrm{MeV}, \alpha \in[-1.8,7.8]$

## Conclusions

- $D_{\text {ov-HF }}$ provides better locality than $D_{\text {ov-W }} \rightarrow$ applicable on coarser lattices
- Rotation symmetry improved

Scaling promising (toy models, preliminary QCD results), under investigation

- $\underline{p \text {-regime }: ~ r e s u l t s ~ f o r ~} m_{\pi}, m_{\rho}, m_{\mathrm{PCAC}}, F_{\pi}$ vs. $m_{q}$ similar to standard overlap $\rightarrow$ independent confirmation, $Z_{A}$ much closer to 1
- $\underline{\epsilon \text {-regime }: ~} \Sigma=(268(2) \mathrm{MeV})^{3}$ from Dirac spectrum
$F_{\pi} \simeq 104( \pm 9) \mathrm{MeV}$ from $\left\langle A_{4} A_{4}\right\rangle$ (preliminary)
agrees exactly with $\chi$ extrapolation from $p$-regime
0 -mode result at $m_{q}=0: \quad F_{\pi}=(80 \pm 14) \mathrm{MeV}, \quad \alpha=-17 \pm 10$
Topology conserving gauge action may be helpful
Thanks to M. Papinutto and C. Urbach for numerical tools

Modified lattice gauge action to "freeze" the topol. sector :
Hernández/Jansen/Lüscher ' 99 , Neuberger '00
Theoretical condition for topology conservation:

$$
\begin{aligned}
S_{P} & :=1-\frac{1}{3} \operatorname{Re} \operatorname{Tr}\left(U_{P}\right)<\varepsilon \simeq 1 / 20.5 \\
U_{P} & : \text { any plaquette }
\end{aligned}
$$

Implementation (Lüscher '01, Fukaya/Onogi '03)

$$
S_{\varepsilon}\left(U_{P}\right)=\left\{\begin{array}{cc}
\frac{S_{P}\left(U_{P}\right)}{1-S_{P}\left(U_{P}\right) / \varepsilon} & S_{P}\left(U_{P}\right)<\varepsilon \\
+\infty & \text { otherwise }
\end{array}\right.
$$

W.B./Jansen/Nagai/Necco/Scorzato/Shcheredin '04
see also Fukaya/Hashimoto/Hirohashi/Ogawa/Onogi, '05

Relax $\varepsilon$, decrease $\beta$ for $\approx$ const. scale, (local HMC)

| $1 / \varepsilon$ | $\beta$ | $r_{0} / a$ | $\beta_{W}$ | $\tau_{\text {aut }}^{\text {top }} / \tau_{\text {aut }}^{\text {plaq }}$ |
| :---: | :---: | :---: | :---: | :---: |
| 0 | 6.18 | $7.14(3)$ | 6.18 | $:=\mathbf{1}$ |
| 1 | 1.5 | $6.6(2)$ | 6.13 | $\sim \mathbf{2 9}$ |
| 1.18 | 1 | $7.2(2)$ | 6.18 | $\sim \mathbf{8 0}$ |
| 1.52 | 0.3 | $7.3(4)$ | 6.19 | $\sim \mathbf{2 4 1}$ |

Approx. const. scale $r_{0} / a$ on a $16^{4}$ lattice
$\beta_{W}$ : corresponding $\beta$ value for the Wilson gauge action
$\tau_{\text {aut }}$ : autocorrelation time with respect to $Q_{\text {top }}$, and to the plaquettes

Allows us to sample a specific top. sector, desired in the $\epsilon$-regime.

Also condition number for $D_{\text {ov }}$ decreases.

