Structure Functions on the Lattice

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- Computation of Matrix Elements
- Non-perturbative Matching
- Summary
The **John von Neumann-Institute of Computing (NIC)**

corporation between **DESY** and **research centre Jülich**

- **NIC** shall provide supercomputer resources

  - centre of Lattice gauge theory **Zeuthen**
  - general computational science **Jülich**

- **NIC** shall maintain research groups
  - *Elementary particle physics* K.J.
  - *Many particle physics* P. Grassberger
Parton distribution functions (PDFs)

- PDFs enter in the calculations of hard processes with hadrons in the initial state and large momentum transfers (DIS, Drell-Yan,...) $x = Q^2/2(pq)$ (Bjorken variable)

- $e^-$: momentum $p$
- $p$: momentum $q$
- $\gamma$: momentum transfer $Q^2$

$$
\sigma = \int_0^1 \sum_f f_f(x, Q^2) \hat{\sigma}(x, Q^2)
$$

- $\hat{\sigma}(x, Q^2)$ hard process $\Rightarrow$ calculable in perturbative QCD

- $f_f(x, Q^2)$ parton distribution function: probability to find parton with momentum fraction $x$ in the proton
Operator product expansion

cross section: \( \sigma \propto W_{\mu\nu}(Q^2) \propto \int d^4y \ e^{iqy} \langle h|j_\mu(y)j_\nu(0)|h\rangle \)

\( W_{\mu\nu}(Q^2) \) hadronic tensor, \( j_\mu(y) \) hadronic current

- In the Bjorken limit \((-q^2 = Q^2 \to \infty, \ x = Q^2/2(pq))\), the region giving the dominant contribution is \( y^2 \simeq 0 \) Light-cone dominance

- Light-cone expansion expresses \( W_{\mu\nu}(Q^2) \) as a sum of local operators times suitable “coefficient functions”

\[
W(Q^2) = \sum_{i,N} C_N^{(i)}(x^2)x^{\mu_1} \cdots x^{\mu_N}O_{\mu_1 \cdots \mu_N}^{(i)}(0)
\]
Moments of PDFs

- The moments of PDF are related to leading twist $\tau$ ($\tau = \text{dim-spin}$) operators of given spin

$$\langle x^N \rangle(\mu) = M_a^{(N)}(\mu^2 = Q^2) = \int_0^1 dx \ x^N [f_f(x, Q^2) + (-1)^{N+1} f_{\bar{f}}(x, Q^2)]$$

via the operator product expansion

$$\sum_f f_f \propto \sigma \propto W \propto O$$

these moments can be represented as expectation values of local operators

$$\langle P | O_{\mu_1 \ldots \mu_N}(0) | P \rangle = M_a^{(N-1)}(\mu) P_{\mu_1} \cdots P_{\mu_n}$$
Experimental situation
→ very precise measurements:
unpolarized structure functions
in a wide kinematic regime

- DESY with HERA
- SLAC
- JLAB
- BNL-RHIC
- Tevatron
- LHC
Global fits

general phenomenological ansatz

\[ x f(x, Q_0^2) = A x^\alpha (1 - x)^\beta \]

⇒ fit to experimental data
⇒ determine the moments of parton distribution functions

Fitting machinery developed: MRST, CTEQ

Very difficult and an art by itself: error determination
Example of comparison with experiment

- Deuteron Spin Structure
  - E155 Collaboration
  - twist-3 matrix element $d_2$
Uncertainties in global fits

Example: gluon uncertainty S. Alekhin, hep-ph/0211096

see also: A.D. Martin et.al. Alekhin, hep-ph/0211080

attempt for direct comparison to lattice data:
Extraction of $\alpha_s$

Experimental evidence (SLAC):

$$F(x, Q^2) \bigg|_{x \approx 0.25, Q^2 > 10 \text{GeV}} \text{ independent of } Q^2$$

→ (Bjorken) scaling

Interpretation (Feynman): scattering on many single partons in a hadron

→ Parton model

→ quarks
Extraction of $\alpha_s$ from scaling violation

perturbative evaluation (NNNLO) of non-singlet parton distribution function

$$\int_0^1 x f(x, Q^2) \frac{dx}{x} = 3 \left[ 1 - \frac{\alpha_s(Q^2)}{\pi} - a(n_f) \left( \frac{\alpha_s(Q^2)}{\pi} \right)^2 - b(n_f) \left( \frac{\alpha_s(Q^2)}{\pi} \right)^3 \right] + \Delta HT$$

- $a(n_f), b(n_f)$ calculable coefficients
- $\Delta HT$ higher twist contributions

⇒ fitting experimental data: extraction of $\alpha_s(Q^2)$

problem: need the full interval in $x$

- model dependence in extrapolation outside experimental data
- singlet contribution very imprecise ← mixing with gluon contribution

⇒ lattice could help substantially
important contribution from deep inelastic scattering

important contribution from lattice calculations
Moments ↔ local operators

Instead of studying the parton distribution functions themselves, we consider scale dependent moments

\[ M_a^{(n)}(\mu) = \int_0^1 dx x^{n-1} f_a(x, \mu) \quad n = 1, 2, \ldots \]

the reason is that the moments can be related to expectation values of local operators \( O_a^n \) suitable for the lattice

\[ M_a^{(n)}(\mu) = \langle O_a^n \rangle \]

\[ \{p^{\mu_1} \cdots p^{\mu_n}\}_{\text{TS}} \langle O_a^n \rangle = \langle p|\bar{\psi}_a(x) \{\gamma^{\mu_1}iD^{\mu_2} \cdots iD^{\mu_n}\}_{\text{TS}} \psi_a(x)|p\rangle \]

- \( \langle p| \) state vector of a hadron with momentum \( p \)
- \( D^\mu \) covariant derivative (gauge invariance)
- TS means to take traceless symmetric part
Examples of Moments

unpolarized quark distributions:

\[ \langle x^n \rangle \sim \langle | \bar{\psi} \gamma_{\mu_1} \cdots D_{\mu_n} \psi | \rangle \]

spin-dependent structure function \( g_1 \):

\[ \langle (\Delta x)^n \rangle \sim \langle | \bar{\psi} \gamma_5 \gamma_{\mu_1} D_{\mu_2} \cdots D_{\mu_n} \psi | \rangle \]

spin-dependent structure function \( g_2 \):

\[ \langle x^n \rangle_{g_2} \sim \langle | \bar{\psi} \gamma_5 [\gamma_{\mu_1} D_{\mu_2}] \cdots D_{\mu_n} \psi | \rangle \]

transversity structure function \( h_1 \):

\[ \langle (\delta x)^n \rangle \sim \langle | \bar{\psi} \gamma_5 \sigma_{\mu_1} D_{\mu_2} \cdots D_{\mu_n} \psi | \rangle \]

unpolarized gluon distribution

\[ \langle x^n \rangle_g \sim \langle h | \sum_{\rho} \text{Tr} (F_\rho \gamma_1 D_{\mu_2} \cdots D_{\mu_n} F_{\rho_1}) | h \rangle \]

latter have been so far quite hard to compute on the lattice
all these moments can be extracted from experimental data
the local operators are to be renormalized

Example: renormalized average momentum (pion) at scale $\mu_0$

$$\langle x \rangle (\mu_0) = \langle \pi | O^{\text{ren}}(\mu_0) | \pi \rangle \equiv \langle \pi | O^{\text{bare}} / Z(\mu_0) | \pi \rangle$$

renormalized average momentum at a different scale

$$\langle x \rangle (\mu) = \langle x \rangle (\mu_0) \cdot \sigma Z(\mu / \mu_0) , \quad \sigma Z(\mu / \mu_0) = \frac{Z(\mu_0)}{Z(\mu)}$$

$\sigma Z(\mu / \mu_0)$ **step scaling function**

**Schödinger functional** renormalization scheme $\rightarrow$ renormalization condition

$$\langle SF | O^R(\mu = 1/L) | SF \rangle = \langle SF | O^{\text{tree}} | SF \rangle$$

with $|SF\rangle$ a Schödinger functional state, i.e. a classical quark at the (time) boundary with an external momentum $p$

in perturbation theory $Z(1/\mu) = 1 - \bar{g}^2(\mu) \left[ \gamma^{(0)} \ln(\mu) + B_0 \right]$ with $\gamma^{(0)}$ the anomalous dimension $B_0$ the constant part
having the running matrix element $\langle x \rangle_{\text{SF}}(\mu)$

$\Rightarrow$ for small enough coupling $\bar{g}$, define the
renormalization group invariant matrix element

$$O_{\text{INV}}^{\text{ren}} = O_{\text{SF}}^{\text{ren}}(\mu) \cdot f_{\text{SF}}(\bar{g}^2(\mu))$$

$$f_{\text{SF}}(\bar{g}^2(\mu)) = (\bar{g}^2(\mu))^{-\gamma_0/2b_0} \exp \left\{ - \int^{\bar{g}(\mu)}_0 dg \left[ \frac{\gamma(g)}{\beta(g)} - \frac{\gamma_0}{b_0 g} \right] \right\}$$

$\gamma(g)$: anomalous dimension function, $\beta(g)$: $\beta$-function

knowing $O^{\text{ren}}$ we can get “easily” the matrix element in a desired scheme

$$\langle x \rangle^{\text{SF}} = O_{\text{INV}}^{\text{ren}} / f_{\text{SF}}(\bar{g}^2(\mu))$$

$$\langle x \rangle^{\text{MS}} = O_{\text{INV}}^{\text{ren}} / f_{\text{MS}}(\bar{g}^2(\mu))$$

$$\langle x \rangle^{\text{my preferred}} = O_{\text{INV}}^{\text{ren}} / f_{\text{my preferred}}(\bar{g}^2(\mu))$$

$\Rightarrow$ make contact with analytical computations in perturbation theory!
How to get $O_{\text{INV}}^{\text{ren}}$?

$$O_{\text{INV}}^{\text{ren}} = O_{\text{SF}}(\mu) \cdot f^{\text{SF}}(\bar{g}^2(\mu)) = \frac{\langle \pi | O_{\text{NS}} | \pi \rangle}{Z^{\text{SF}}(1/\mu)} \cdot f^{\text{SF}}(\bar{g}^2(\mu))$$

$$= \frac{\langle \pi | O_{\text{NS}} | \pi \rangle}{Z^{\text{SF}}(1/\mu_0)} \cdot \frac{Z^{\text{SF}}(1/\mu)}{Z^{\text{SF}}(1/\mu)} \cdot f^{\text{SF}}(\bar{g}^2(\mu))$$

$$\equiv \sigma(\mu/\mu_0, \bar{g}(\mu))$$

$$\equiv O_{\text{SF}}^{\text{ren}}(\mu_0) \sigma(\mu/\mu_0, \bar{g}(\mu)) \cdot f^{\text{SF}}(\bar{g}^2(\mu))$$

$$\equiv \mathcal{G}_{\text{UV}}^{\text{INV}}(\mu_0)$$

- $O_{\text{SF}}^{\text{ren}}(\mu_0)$ renormalized matrix element → only to be computed once
- $\sigma(\mu/\mu_0, \bar{g}(\mu))$ step scaling function
- $\mathcal{G}_{\text{INV}}^{\text{UV}}(\mu_0)$ (ultraviolett) renormalization group invariant step scaling function

$O_{\text{INV}}^{\text{ren}} = O_{\text{SF}}^{\text{ren}}(\mu_0) \mathcal{G}_{\text{INV}}^{\text{UV}}(\mu_0)$
Summary

- Parton distribution functions are determined very precisely in experiments worldwide.
- They provide important information about the spin structure of hadrons and may give very precise value of $\alpha^2$.
- Further our understanding of QCD or shed light on new physics.
- Important: also moments of parton distribution functions can be determined from experiment.
  - Accessible to lattice computations.
  - Need scale dependent renormalization.
- Most important theoretical quantity: renormalization group invariant matrix element.
\( Z \) can be computed in practice by calculating fermion correlation functions in the Schrödinger functional set up

consider a correlation function \( f_O \) of our operator \( O \)
at a distance \( x_0/L \) fixed (e.g. \( x_0/L = 1/2 \))

\[
f_{\bar{Z}}(x_0) = \sum_{y,z} e^{i p(y-z)} \langle \bar{\psi}(x) O \tau^3 \psi(x) \bar{\zeta}(y) \frac{1}{4} \tau^a \zeta(z) \rangle
\]

with some choice of the momentum \( p \) and \( \Gamma = \gamma_2 \)

\( \zeta, \bar{\zeta} \) are boundary quark fields at \( x_0 = 0 \)

the desired value of \( \bar{Z} \) is then obtained by normalizing with \( f_{\bar{Z}}^{\text{tree}}(x_0) \)

\[
\bar{Z}(L) = \frac{f_{\bar{Z}}(x_0)}{f_{\bar{Z}}^{\text{tree}}(x_0)} \bigg|_{x_0/L = \text{fixed}}
\]
→ need normalization of boundary fields

\[ f_1 = -\frac{1}{L^6} \sum_{u,v,y,z} \frac{1}{3} \langle \tilde{\zeta}'(u) \Gamma \frac{1}{4} \tau^3 \tilde{\zeta}'(v) \tilde{\zeta}(y) \Gamma \frac{1}{4} \tau^3 \zeta(z) \rangle \]

definition of the normalization constant

\[ Z(L) = \frac{\tilde{Z}(L)}{\sqrt{f_1(L)}} \]

and we have the step scaling functions

\[ \sigma_{\tilde{Z}} = \frac{\tilde{Z}(2L)}{Z(L)}, \sigma_{f_1} = \frac{\sqrt{f_1(2L)}}{\sqrt{f_1(L)}}, \sigma_Z = \frac{Z(2L)}{Z(L)} \]

→ note that so far the who discussion was in the continuum!
Excursion to the lattice

non-perturbative information from numerical simulations

→ make \( Z(\mu) \) dependend on the lattice spacing

\[
Z(\mu) = Z(\mu, a)
\]

the lattice step scaling function is then (step size \( s \))

\[
\Sigma_Z(a) = \frac{Z(sL,a)}{Z(L,a)}
\]

\( s \) usually taken to be 2

aim: continuum limit (\( \exists \) for \( \Sigma_Z \)):

\[
\sigma_Z = \lim_{a \to 0} \Sigma_Z(a)|_{\mu^{-1}=L \text{ fixed}}
\]

how do we fix the scale?

→ through the coupling constant \( g = \bar{g}(\mu = 1/L) \)

(computation of running coupling necessary prerequisite)
continuum limit is reached through a matching procedure

\[ \bar{g}^2(L) \text{ fixed} \]

\[ Z(L) \]  \[ \rightarrow \]  \[ Z(2L) \]

\[ a = 0.25\text{fm} \]

\[ a = 0.125\text{fm} \]
physical scales in the problem

- lattice extent $L$
- lattice momentum $p = k2\pi/L$, $k = 0, \cdots, L/a - 1$
- time $x_0$ distance from the boundary at $T = 0$
- quark mass $m = 0$ ← Schrödinger functional boundary conditions

then the normalization constant is a function of *dimensionless quantities*

$$Z = Z(pL, x_0/L, a/L)$$

if we only want to change the scale, identified as $\mu^{-1} = L$, we have to keep

$$pL, x_0/L \text{ fixed}$$

while tuning $a/L \to 0$ to reach the continuum limit:

- $pL = 2\pi$ (lowest momentum), $x_0/L = 1/2$
Strategy

- Compute $\langle x \rangle (\beta)$ between pion states in “infinite volume” with $\beta(a)$ given by $r_0$ fixed

- Compute $Z(\beta, \mu_0)$ with $\mu_0^{-1} = 2L_m = 1.4r_0$
  $\Rightarrow$ take continuum limit of $\langle x \rangle (\beta)/Z(\beta, \mu_0)$

- Evolve (step scaling function) from large $L$ (low $\mu$) to small $L$ (high $\mu$)

- Continue with perturbative evolution to arrive at (scale and scheme independent) RGI matrix element

- Connection with experiment evolving in the $\overline{\text{MS}}$ scheme
\[ \langle x \rangle_{RGI} \quad \leftarrow \quad \langle x \rangle_{RGI} \]
\[ \downarrow \quad \uparrow \quad \text{perturbative evolution} \]
\[ \downarrow \quad \uparrow \quad \langle x \rangle_{\overline{MS}} \text{ at } \mu = 2 \text{ GeV} \]
\[ \downarrow \quad \uparrow \quad \langle x \rangle_{SF} \text{ at } L = 0.005 \text{ fm} \]
\[ \uparrow \quad \text{non-perturbative evolution} \]
\[ \uparrow \quad \text{finite-volume scheme} \]
\[ \text{hadronic scheme} \quad \rightarrow \quad \langle x \rangle_{SF} \text{ at } L = 0.7 \text{ fm} \]
Generalized boundary conditions in space

boundary conditions for fermions in spatial directions

$$\psi(x + L \hat{k}) = e^{i\theta_k} \psi(x), \; \bar{\psi}(x + L \hat{k}) = e^{-i\theta_k} \bar{\psi}(x), \; k = 1, 2, 3, \; 0 \leq \theta_k \leq 2\pi$$

implementation in the definition of the gauge covariant lattice derivatives:

$$\nabla_\mu \psi(x) = \frac{1}{a} [\lambda_\mu U(x, \mu) \psi(x + a \hat{\mu}) - \psi(x)]$$

$$\nabla_\mu^* \psi(x) = \frac{1}{a} [\psi(x) - \lambda_\mu^* U(x - a \hat{\mu}, \mu) \psi(x - a \hat{\mu})]$$

$$\lambda_\mu = e^{ia\theta_\mu / L}, \; 0 \leq \theta_k \leq 2\pi, \; \theta_4 = 0,$$

factor $e^{ia\theta_k / L}$ can be interpreted as an external momentum with continuous values
Two representations of twist-2, non-singlet operator on the lattice

\[ O_{12}(x) = \frac{1}{4} \bar{\psi}(x) \gamma_1 \overleftrightarrow{D_2} \frac{1}{2} \tau^3 \psi(x) \]

\[ O_{44}(x) = \frac{1}{2} \bar{\psi}(x) \left[ \gamma_4 \overleftrightarrow{D_4} - \frac{1}{3} \sum_{k=1}^{3} \gamma_k \overleftrightarrow{D_k} \right] \frac{\tau^3}{2} \psi(x). \]

external momentum \( \rightarrow \theta_k \)

\[ \theta \equiv \theta_1 \neq 0, \ \theta_2 = \theta_3 = 0 \]

\( \theta \) appears in derivative and in propagators
Correlation functions at tree level
Choice of $\theta$

- convergence of perturbation theory, i.e. the values of the anomalous dimensions
- cut-off effects
- signal to noise ratio
Perturbation Theory

perturbative expansion

\[
Z_\mathcal{O}(g_0, a/L, x_4/L, \theta) = 1 + \sum_{k=1}^{\infty} Z^{(k)}_\mathcal{O}(a/L, x_4/L, \theta) g_0^{2k},
\]

for \(a/L \to 0\) coefficients \(Z^{(k)}_\mathcal{O}\) are polynomials in \(\ln(L/a)\) of degree \(k\) up to corrections of \(\mathcal{O}(a/L)\)

1-loop:
\[
Z^{(1)}_\mathcal{O} = B_\mathcal{O}(\theta, x_4/L) - \gamma_0 \ln(L/a) + \mathcal{O}(a/L).
\]

2-loop coefficient \(\gamma_1\) in SF-scheme can be obtained by knowing 2-loop coefficient in a different scheme

\[
\gamma_1 = \gamma_1^{\overline{\text{MS}}} + 2b_0 \Delta Z^{(1)}_\mathcal{O} - \gamma_0 \mathcal{X}^{(1)}_g
\]

\(\Delta Z^{(1)}_\mathcal{O}\) 1-loop difference of renormalization constants

\(\mathcal{X}^{(1)}_g\) relation of renormalized coupling in two schemes

*if wanted, this can be explained*

Goal: \(\gamma_0/\gamma_1 \ll 1\)
Relating Schemes

A matrix element $O^s_R$ renormalized in a certain scheme $s$ is obtained by

$$O^s_R = Z^{s,\text{reg}} O^{\text{reg}}_b$$

$O^{\text{reg}}_b$ is bare matrix element computed within a certain regularization $\text{reg}$
$Z^{s,\text{reg}}_O$ depends on the renormalization scheme $s$ used and on the regularization $\text{reg}$

Operators renormalized in two different schemes but using the same regularization can be related by a finite renormalization

$$O^s' = O^s \Delta Z^{s'}_O \leftarrow s$$

$\Delta Z^{s'}_O \leftarrow s$ is independent from the regularization used to compute the renormalized matrix element and the corresponding renormalization constant

in principle it is possible to compute anomalous dimension and finite part in the SF scheme, using the dimensional regularization

→ connect directly with the $\overline{\text{MS}}$ scheme
Relating Schemes

connect directly with the $\overline{\text{MS}}$ scheme

$$\Delta Z^{SF\leftarrow \overline{\text{MS}}} = \frac{Z^{SF,DR}}{Z^{\overline{\text{MS}},DR}_O}$$

However, $Z^{SF,DR}_O$ not known $\Rightarrow$ bridge via the MOM-scheme

the desired factor $\Delta Z^{SF\leftarrow \overline{\text{MS}}} = \Delta Z^{SF\leftarrow \text{MOM}} \Delta Z^{\text{MOM}\leftarrow \overline{\text{MS}}}$.\]

two factors $\Delta Z$ are computed using different regularizations:
$\Delta Z^{SF\leftarrow \text{MOM}}$ computed on the lattice
$\Delta Z^{\text{MOM}\leftarrow \overline{\text{MS}}}$ in dimensional regularization

using the complete one loop result in the MOM scheme which exists in both, lattice and dimensional, regularizations, it is then possible to compute $\Delta Z^{(1)}_O$ and from this finally $\gamma_1$
Relating Schemes

Renormalization schemes

Lattice reg.  Dimensional reg.

SF  MS  MOM
Perturbative renormalization group functions

\[ \beta(g) = \mu \frac{\partial}{\partial \mu} g(\mu) \]

\[ \gamma(g) = \mu \frac{\partial}{\partial \mu} \log Z_O(\mu, g) \]

have asymptotic expansions of the form

\[ \beta(g) \overset{g \to 0}{\sim} -g^3 \sum_{k=0}^{\infty} b_k g^{2k}, \quad \gamma(g) \overset{g \to 0}{\sim} -g^2 \sum_{k=0}^{\infty} \gamma_k g^{2k} \]

\[ C_F = (N_c^2 - 1)/2N_c \] and \( N_c \) the number of colors

\[ b_0 = \left\{ \frac{11}{3} N_c - \frac{2}{3} N_f \right\} (4\pi)^{-2} \]

\[ \gamma_0 = \frac{16}{3} C_F (4\pi)^{-2} \]

\[ b_1 = \left\{ \frac{34}{3} N_c^2 - \left( \frac{13}{3} N_c - N_c^{-1} \right) N_f \right\} (4\pi)^{-4} \]
Any two mass independent renormalization schemes can be related by a scale change and a finite parameter renormalization of the form

\[ \mu' = c \mu, \quad c > 0 \]
\[ g' = g \sqrt{X_g(g)} \]
\[ Z' = Z[\Delta Z_O(g)], \]
\[ X_g(g) \xrightarrow{g \to 0} 1 + \sum_{k=1}^{\infty} X_g^{(k)} g^{2k}. \]
\[ \Delta Z_O(g) \xrightarrow{g \to 0} 1 + \sum_{k=1}^{\infty} \Delta Z_O^{(k)} g^{2k}. \]

The invariance of a physical observable under such a change of parameters, gives a relation between the renormalization group functions, \( \beta \) and \( \gamma \), in the 2 schemes. In particular we have

\[ \gamma_1 = \gamma_{1 \overline{\text{MS}}} + 2b_0 \Delta Z_O^{(1)} - \gamma_0 X_g^{(1)} \]
\[ X_g^{(1)} = -\frac{1}{4\pi} (c_{1,0} + c_{1,1} N_f) \]
\[ c_{1,0} = 1.25563(4), \quad c_{1,1} = 0.039863(2) \]
### Anomalous dimensions

<table>
<thead>
<tr>
<th>$\theta$</th>
<th>$\gamma_1^A(\theta)$</th>
<th>$\gamma_1^B(\theta)_{2,b}$</th>
<th>$\gamma_1^A(\theta)/\gamma_0$</th>
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<td>$-$0.7578(6)</td>
</tr>
</tbody>
</table>

**Table 1:** 2-loop anomalous dimension for the $O_{44}$ representation
Cutoff effects in Perturbation Theory

define perturbative step scaling function $k(a/L; x_4/L, \theta)$

$$k(a/L; x_4/L, \theta) = Z_{\mathcal{O}}^{(1)}(a/2L; x_4/L, \theta) - Z_{\mathcal{O}}^{(1)}(a/L; x_4/L, \theta).$$

deviation from continuum value $k(0; x_4/L, \theta) = -\gamma_0 \ln(2)$
Signal to Noise Ratio

\[ \Delta \frac{Z}{Z} \]

Relative error \( \Delta \frac{Z}{Z} \)
Cutoff effects in Step Scaling Function

Start simulation with pure Wilson fermions (and Wilson plaquette action)
Cutoff effects in Step Scaling Function

large cutoff effects
non-monotonic behaviour
extrapolation trustworthy?
solution: perform simulation with two formulations of lattice fermions

- Wilson fermions
- full $O(a)$ non-perturbatively improved Wilson fermions

for complete $O(a)$ improvement we would need also the operator to be improved, giving the form

$$O_{\text{impr}} = c_1 \bar{\psi} \gamma_\mu D_\nu \psi + c_2 \bar{\psi} \sigma_{\mu\nu} F_{\mu\nu}$$

$$+ c_3 \bar{\psi} \{D_\mu, D_\nu\} + c_4 \partial_\lambda (\bar{\psi} \sigma_{\mu\lambda} D_\nu)$$

⇒ complicated operator and difficult to determine the coefficients $c_1, \ldots, c_4$
non-perturbatively

→ attempt to first only improve the action

→ provides a check on the continuum extrapolation of $\sigma$
Cutoff effects in Step Scaling Function

- pure Wilson
- $O(a)$ improved Wilson

$\sigma_{f_1}$ for improved Wilson

no cutoff effects ← expected compatible continuum values

$\bar{g}^2 = 2.45$
Combined, constraint continuum extrapolation

\[ \sigma_{\tilde{z}} \]

\[ a/L \]

- \ldots pure Wilson
- \textcolor{red}{O(a)} improved Wilson

check on continuum extrapolation
Step Scaling Function in the Continuum

The parametrization is given by:

\[ \sigma_{Z_{12}} = 1 - \gamma_0 \ln(2)g_0^2 + c_1g_0^4 + c_2g_0^6 \]
Renormalization Group Invariant Step Scaling Function

$$\Theta_{\text{INV}}^{\text{UV, SF}}(\mu_0) = \sigma(\mu/\mu_0, \bar{g}^2(L_0)) \cdot (\bar{g}^2(L))^{-\gamma_0/2b_0} \exp \left\{ - \int_0^{\bar{g}(\mu)} dg \left[ \frac{\gamma(g)}{\beta(g)} - \frac{\gamma_0}{b_0g} \right] \right\}$$

need step scaling function in steps of two ⇒ interpolation in $g_0$

be careful with error propagation:

$$(\Delta \sigma_{Z\phi}) = \sqrt{\frac{\partial \sigma_{Z\phi}}{\partial c_1}^2 (\Delta c_1)^2 + \frac{\partial \sigma_{Z\phi}}{\partial c_2}^2 (\Delta c_2)^2 + 2 \frac{\partial \sigma_{Z\phi}}{\partial c_1} \cdot \frac{\partial \sigma_{Z\phi}}{\partial c_2} \cdot \text{cov}_{12} + \frac{\partial \sigma_{Z\phi}}{\partial \bar{g}^2} \Delta \bar{g}^2}$$
Renormalization Group Invariant Step Scaling Function

\[ \Lambda^{(0)}_{\text{SF}} \approx 120 \text{ MeV} \]
being the \( \Lambda \)-parameter
in the quenched approximation
in the SF scheme
use 3-loop \( \beta \)-function
use 2-loop \( \gamma \)-function

\[ S_{\text{UV, SF}}^{\text{INV}, \mathcal{O}_{12}}(\mu_0) = 0.242(8), \quad S_{\text{INV, SF}}^{\text{UV}, \mathcal{O}_{44}}(\mu_0) = 0.221(9). \]
Summary II

- Schrödinger Functional well suited to determine step scaling function

- generalized boundary conditions in space offer new handle to optimize the simulations

- determination of renormalization group invariant step scaling function possible in the continuum
The Matrixelement

\[ \lim_{a \to 0} \frac{\langle \pi | O_2 | \pi \rangle}{Z_{O_2}(L_0)} \bigg|_{m_q=0} \]

to determine \( Z(L_0) \) keep fixed the scale \( \mu_0^{-1} = L_0 = 0.7 \cdot r_0 \) (\( r_0 = 0.5 \text{fm} \))

choose a sequence of lattices \( N = L_0/a \) such that \( a \to 0 \) while \( \bar{g}^{SF}(1/L_0) \) fixed

\( \Rightarrow \) fine adjustment of \( \beta = 6/g_0^2 \)
use $SF$ to compute the matrix element

while sending $a \rightarrow 0$

- time extent $T = 3\text{fm}$ fixed
- time distance from boundary fixed to be $1\text{fm}$ → sufficient to project on pion state
- keep plateau length for extracting the matrix element fixed to be $1\text{fm}$
Finite Size Effects

We will consider the example of a twist-2 non-singlet operator in pion states

\[ \mathcal{O}_{44}(x) = \frac{1}{2} \bar{\psi}(x) \left[ \gamma_4 \vec{D}_4 - \frac{1}{3} \sum_{k=1}^{3} \gamma_k \vec{D}_k \right] \psi(x) \]

\[ S = \frac{a^6}{L^3} \sum_{y,z} \bar{\zeta}(y) \gamma_5 \tau^+ \zeta(z), \quad S' = \frac{a^6}{L^3} \sum_{u,w} \bar{\zeta}'(u) \gamma_5 \tau^- \zeta'(w) \]

Consider then the correlation functions

\[ f_{44}(x_0) = \langle S\mathcal{O}_{44}(x)S' \rangle \]

\[ f_{1} = -\frac{1}{2} \langle SS' \rangle \]

quantum mechanical interpretation

\[ f_{44}(x_0) = \mathcal{Z}^{-1} \langle i_{\pi} | e^{-(T-x_0)\mathcal{H}} P \mathcal{O}_{44}(x) e^{-x_0\mathcal{H}} P | i_{\pi} \rangle, \quad f_{1} = \mathcal{Z}^{-11} \langle i_{\pi} | e^{-THF} P | i_{\pi} \rangle \]

\( P \) projector on gauge invariant states
**Finite Size Effects**

Inserting a complete set of eigenstates of the hamiltonian

- correlation function

\[ f_A(x_0) \simeq \rho^2 e^{-m_\pi x_0} \left\{ 1 + \eta e^{-x_0 \Delta} + \eta' e^{-(T-x_0)m_G} \right\} \]

pion gap: \( \Delta r_0 \approx 3.2 \quad 0^{++} \text{mass : } m_{G} r_0 \approx 4.3 \)

- matrix element

\[ f_{44}(x_0) \simeq \rho^2 \langle 0, \pi | \mathcal{O}_{44}(x) | 0, \pi \rangle e^{-m_\pi T} \left\{ 1 + \eta^\pi \mathcal{O}_{44} e^{-x_0 \Delta} + \eta'^\pi \mathcal{O}_{44} e^{-(T-x_0)\Delta} \right\} \]

- boundary to boundary correlation function

\[ f_1 \simeq \rho^2 e^{-m_\pi T} \]

\[ \frac{f_{44}(x_0)}{f_1} = \langle 0, \pi | \mathcal{O}_{44}(x) | 0, \pi \rangle + \text{exc.st.} \]
Effective masses and plateau

effects form excited states,

\[ m_{\text{eff}}(x_0) \approx m_\pi + \Delta \eta^\pi_A e^{-\Delta x_0} - m_G \eta^0_A e^{-m_G (T-x_0)} \]

\[ \langle x \rangle (x_0) \approx \langle x \rangle \left\{ 1 + \eta_{\pi M} (e^{-\Delta x_0} + e^{-\Delta (T-x_0)}) \right\} \]

pion gap: \( \Delta r_0 \approx 3.2 \)

0\(^{++}\) mass: \( m_G r_0 \approx 4.3 \)

choose corrections \( \Delta \eta^\pi_A e^{-\Delta x_0} \) and \( -m_G \eta^0_A e^{-m_G (T-x_0)} \) small

⇒ choose value of \( x_0 \) large enough to read off effective masses and plateaus for matrix element
Finite Size Effects

\[ m_{\text{eff}} e^{-\Delta x_0} e^{-m_{\text{G}} (T-x_0)} \]

→ corrections consistent with estimate of higher state contributions
Finite Size Effects

Examples for $\beta = 6.45$, $32^3 \times 72$ lattice

$\Rightarrow$ read off plateau by demanding that effects of higher states are less than 0.001

$\Rightarrow$ fit range

$1.2 \text{ fm} \leq x_0 \leq 2.4 \text{ fm}$  $m_{\text{eff}}$  $1.3 \text{ fm} \leq x_0 \leq 2.2 \text{ fm}$ matrix element
Finite Size Effects

Finite volume effects for pion mass:

\[ m_\pi(L) = c_0 + \frac{c_1}{L^{3/2}} \exp(-c_2L) \]

\[ \rightarrow \text{no effects for lattice sizes larger than } L \approx 1.2 \text{ fm and } T \approx 2.8 \text{ fm} \]
Finite Size Effects

Finite volume effects for the pion matrix element:

- **Power law**
  \[ \langle x \rangle(L) = c_0 + \frac{c_1}{L^{c_2}} \]

- **Exponential**
  \[ \langle x \rangle(L) = c_0 + \frac{c_1}{L^{3/2}} \exp \left( -c_2 L \right) \]

→ large volumes \( L \approx 1.9 \) fm and \( T \approx 3.3 \) fm needed

⇒ warning for nucleon matrix elements
Finite Size Effects

pion mass: $m_\pi L > 4$ sufficient

matrix element: need $m_\pi L > 5$
very good signal for $\theta = 1$
(for $\theta = 0$ or $\theta = 2\pi$ operator would have been very difficult to measure)

\[
\mathcal{O}_{44}(x) = \bar{\psi}(x)\gamma\{4 \rightarrow D_4\} \frac{1}{2}\tau^3 \psi(x)
\]

note the operator $\mathcal{O}_{12}(x) = \bar{\psi}(x)\gamma\{1 \rightarrow D_2\} \frac{1}{2}\tau^3 \psi(x)$ needs an external momentum to saturate indices $\Rightarrow$ very noisy
continuum limit of renormalized matrix element

\[
\langle x \rangle_{\text{SF}}(\mu_0) = \lim_{a \to 0} \left. \frac{\langle \pi | O_2 | \pi \rangle}{Z_{O_2}(L_0)} \right|_{m_q=0}
\]

- use two action method to check for universal continuum limit

linear chiral extrapolation

\[
\langle x \rangle_{\text{SF}}(\mu_0) = \lim_{a \to 0} \lim_{\text{chiral}} \frac{\langle \pi | O_{\text{NS}}^{n=2} | \pi \rangle}{Z_{\text{SF}}(1/\mu_0)} = 0.870(33)
\]
\[ \langle x \rangle_{\text{RGI}} = \langle x \rangle_{\text{SF}}^{\text{ren}}(\mu_0) \mathcal{G}^{\text{UV}}_{\text{INV}}(\mu_0) \]

\[ = 0.870(33) \times 0.221(9) = 0.192(11) \]

Simple conversion to any desired scheme (e.g. \( \overline{\text{MS}} \)):

\[ \langle x \rangle_{\overline{\text{MS}}}^{\overline{\text{MS}}} (\mu = 2 \text{ GeV}) = \langle x \rangle_{\text{RGI}}^{\overline{\text{MS}}} / \mathcal{F}^{\overline{\text{MS}}} (\bar{g}^2(\mu = 2 \text{ GeV})) \]

\[ = 0.265(15) \]

→ Limitation: quenched approximation
renormalization group invariant matrix element

- NLO analysis of Drell-Yan and prompt photon $\pi N$ data (NA10 and E615 collaboration)
  
  SMRS, PRD 45 (1992) 2349

- lattice result evolved in perturbation theory using the RGI matrix element
Summary III

- Schrödinger Functional is also well suited to determine matrix elements
- determine continuum matrix element at a small scale $\mu_0$
- determination of renormalization group invariant matrix element
  - relation to $\overline{\text{MS}}$ scheme
  - comparison to experiment
- method can be used also for hadrons
- method can be used for many more operators
- perturbative analysis of gluon operator available
Quantum chromodynamics

massless QCD has chiral symmetry

\[ \psi \rightarrow e^{i\theta \gamma_5} \psi, \quad \bar{\psi} \rightarrow \bar{\psi} e^{i\theta \gamma_5} \]

or, equivalently, \[ \gamma_5 D_{\text{cont}} + D_{\text{cont}} \gamma_5 = 0, \quad D_{\text{cont}} \] Dirac operator

assuming that chiral symmetry is spontaneously broken and

\[ \langle \bar{\psi} \psi \rangle \neq 0 \]

a number of consequences follow, e.g.

- Goldstone modes = pions (having very small mass)
- low energy relations (PCAC) relying on symmetry arguments alone

description possible by chiral perturbation theory for low energy phenomena in QCD
Chiral symmetry on the lattice

one of our main problems with the lattice is the question of *chiral symmetry*

the problem is *how to have right massless spectrum on the lattice* and preserve continuum chiral symmetry

⇐ impossible due to Nielsen-Ninomiya theorem (Nielsen and Ninomiya) (while keeping also locality)

for Wilson fermions → demonstration in perturbation theory (although in all orders) that *in the continuum limit* chiral symmetry is restored (Bochiccio, Maiani, Rossi, Testa)

non-perturbatively: . . . to be proven
Ginsparg-Wilson relation

\[
\gamma_5 D + D \gamma_5 = 2aD \gamma_5 D
\]

\[
\Rightarrow D^{-1} \gamma_5 + \gamma_5 D^{-1} = 2a \gamma_5
\]

\(D^{-1}\) anti-commutes with \(\gamma_5\) at all non-zero distances

\[\rightarrow\] only mild (i.e. local) violation of chiral symmetry

Ginsparg and Wilson arrived at this expression already in the early days of lattice gauge theories from a completely different path \(<\) block spinning from the continuum

one solution of GW relation: overlap operator \(D_{ov}\) (Neuberger)
(alternatives: domain wall fermions and perfect actions)

\[
D_{ov} = \left[ 1 - A(A^\dagger A)^{-1/2} \right]
\]

with \(A = 1 + s - D_w\) \(s\) a tunable parameter, \(0 < s < 1\)
Moreover: *Ginsparg-Wilson relation* implies an *exact lattice chiral symmetry* (Lüscher):

for any operator $D$ which satisfies the Ginsparg-Wilson relation, the action

$$S = \bar{\psi} D \psi$$

is invariant under the transformations

$$\delta \psi = \gamma_5 (1 - \frac{1}{2} aD) \psi$$
$$\delta \bar{\psi} = \bar{\psi} (1 - \frac{1}{2} aD) \gamma_5$$

⇒ have a notion of chiral symmetry on the lattice

$$\gamma_5 \rightarrow \gamma_5 (1 - \frac{1}{2} aD)$$

the *lattice* operator $D$ enjoys many properties of the *continuum* operator:

$Z_A = Z_V = 1$, anomaly, index theorem, …
in addition:

despite the term \( 1/\sqrt{A^\dagger A} \)

(\( \Rightarrow \) all lattice points are coupled among each other)

the operator \( D_{ov} \) is local, \( \| D_{ov} \Phi \| \propto e^{-\gamma/a} \)

(Hernandèz, Lüscher, K.J.)

• if plaquette is bounded: \( \| 1 - U_P \| < 1/30 \)
  (analytical proof)

• locality also demonstrated numerically when bound not satisfied

\( \Rightarrow \)

• *chiral symmetric*

• *local*

lattice QCD \( \rightarrow \) non-perturbative definition of QCD \( (a \rightarrow 0) \)
one of the major **assumptions** in QCD is that chiral symmetry is spontaneously broken by the formation of a scalar condensate $\langle \bar{\psi} \psi \rangle$

spontaneous breaking of chiral symmetry

$\Rightarrow$ appearance of **Goldstone particles** (pions) *(Goldstone theorem)*

$\Rightarrow$ many low energy relation *(PCAC relation)* in QCD

$\Rightarrow$ application of chiral perturbation theory

*the lattice is a unique environment to test this basic assumption and an operator satisfying the Ginsparg-Wilson relation provides the necessary tool to perform this test in practice*
simulations with overlap fermions $\gg$ more expensive than standard fermions $\Rightarrow$ use quenched approximation

results for scalar condensate $\Sigma(m, V)$ as function of quark mass $m$ and volume $V$ in quenched chiral perturbation theory has been worked out (Damgaard, Osborn, Toublan, Verbaaschoot)

$$\Sigma(m, V) = \Sigma \sum z [I_{\nu}(z)K_{\nu}(z) + I_{\nu+1}(z)K_{\nu-1}(z)] + \Sigma_{\nu}^{V}$$

$z = m\Sigma V$, $\nu$ denotes the topological charge sector
$\Sigma$ infinite volume, chiral limit scalar condensate

for $m \to 0$ approximate formulae are obtained

$$\Sigma_{\nu=0}(a) = m \Sigma^2 V \left(1/2 - \gamma + \ln 2 - \ln m\Sigma V + O(m\Sigma V)^2\right)$$

$$\Sigma_{\nu=\pm 1}(a) = \frac{1}{mV} + \frac{1}{2}m\Sigma^2 V \left(1 + O(m\Sigma V)^2\right)$$

at finite lattice spacing $a$ there is a quadratic divergence $\propto 1/a^2$

this divergence has to be subtracted (i.e. fitted)
Computation of chiral condensate using overlap fermions

data points at 7 masses on 3 volumes
attempt a fit according to

$$\Sigma_{\nu=\pm 1} = \Sigma z \left[ I_{\nu}(z) K_{\nu}(z) + I_{\nu+1}(z) K_{\nu-1}(z) \right] + C/a^2$$

→ only two free parameters
$\Sigma$ and $C$

(Hernández, Lellouch, K.J.)

⇒ find strong evidence for spontaneous chiral symmetry breaking in QCD!
Systematic uncertainties of $\langle \bar{\psi} \psi \rangle$:

i) have only computed bare $\langle \bar{\psi} \psi \rangle$
   → *non-perturbative* renormalization

$$\langle \bar{\psi} \psi \rangle_{\text{ren}} = \langle Z(\mu) \bar{\psi} \psi \rangle + \frac{c_1}{a^3} + m_q \frac{c_2}{a^2} + m_q^2 \frac{c_3}{a}$$

- $c_1$ exactly known for Ginsparg-Wilson fermions
- $c_2$ subtracted non-perturbatively
- $c_3$ neglected since $m_q \ll 1$
  
  *(data: term negligible)*

- $Z(\mu)$ scale $\mu$ dependent renormalization factor

ii) only one value of the lattice spacing
    → need continuum extrapolation

iii) quenched approximation
    → include effects of dynamical quarks
renormalization factor $Z(\mu)$

in principle: need a box covering all energy scales

$$a \ll \frac{0.001\text{fm}}{\text{MW}} - \frac{1\text{fm}}{\text{conf.scale}} < L$$

$\Rightarrow$ huge and unrealistic number of lattice points $N^4$

solution: **Finite size scaling** method, breaking the problem up into many smaller steps

$\rightarrow$ very expensive with the overlap operator

$\rightarrow$ method needs special boundary conditions: implementation not known for overlap operator

way out: *matching of different lattice regularizations*

for $O(a)$-improved Wilson fermions the quark mass renormalization factor $Z_m(\mu)$ is known
Renormalization factors from matching conditions

P. Hernández, K.J., L. Lellouch and H. Wittig,
JHEP 0107 (2001) 018, hep-lat/0106011; hep-lat/0110199

→ fix physical situation: choice \((r_0 M_P)^2 = x_{\text{ref}}\) fixed

⇒ match renormalization group invariant (RGI) quantities

- RGI quark mass \(M = Z_M(g_0) m(g_0)\)
  - \(m\) current quark mass
    (=bare quark mass for overlap fermions)

- RGI matrixelement of pseudoscalar density \(G_P^{\text{RGI}} = Z_P(g_0) G_P(g_0)\), \(G_P = \langle 0|P|PS\rangle\)

matching conditions (hold true in the continuum)

\[
Z_{M}^{ov}(g_0) m_{ov}^{ov}(g_0) = Z_{M}^{w}(g_0) m_{w}^{w}(g_0) \bigg|_{x_{\text{ref}}}
\]

\[
Z_{P}^{ov}(g_0) G_{P}^{ov}(g_0) = Z_{P}^{w}(g_0) \frac{\bar{m}}{M} G_{P}^{w}(g_0) \bigg|_{x_{\text{ref}}}
\]
why is this helpful for renormalizing $\langle \bar{\Psi} \Psi \rangle$?

→ for chiral invariant formulations

$$Z_S = Z_P = \frac{1}{Z_M}$$

putting in a physical scale

$$Z_{m}^{ov}(g_0) = \left. \left( \frac{Z_{m}^{wil}(g_0)(r_0 m_{wil})(g_0')}{(r_0 m_{ov})(g_0)} \right) \right|_{(r_0 m_P)^2=x_{ref}}$$

- $r_0 = 0.49\text{fm}$ hadronic radius
continuum limit for Wilson part can be taken
data exist in literature
J. Garden, J. Heitger, R. Sommer, H. Wittig, Nucl.Phys.B571 (200) 237

\[ U_M = \lim_{g'_0 \to 0} \left\{ Z_{m\text{wil}}^{w}(g'_0)(r_0m_{\text{wil}})(g'_0) \right\} \bigg|_{x_{\text{ref}}} \]

similar a \( U_P \) for the pseudoscalar matrix element can be computed

\[ U_P = \lim_{g'_0 \to 0} \left\{ Z_{P}^{w}(g'_0)\bar{m}^{\text{SF}}_{M} \times (1 + a b_P m_q) (r_0^2G_{P}^{w})(g'_0) \right\} \bigg|_{x_{\text{ref}}} \]

\( b_P \) improvement coefficient

\( \Rightarrow \) only remaining lattice artefacts from overlap fermions

\( \Rightarrow \) check on scaling behaviour fermions
⇒ knowing $Z_m^{ov}(g_0)$ and $\Sigma_{bare}(g_0)$

define a renormalization group invariant scalar condensate

$$\hat{\Sigma} = \frac{1}{Z_m^{ov}(g_0)} \Sigma_{bare}(g_0)$$

knowing $\hat{\Sigma}$

→ scale dependence of the quark condensate in any scheme:

→ integrate the perturbative renormalization group function (known up to four loops)
$f(\mu)$ in the corresponding scheme

$$\Sigma_{ren}(\mu) = f(\mu) \hat{\Sigma}$$

⇒ obtain a fully renormalized quark condensate
Pseudoscalar mass for overlap and Wilson fermions

→ linear dependence of $m_P^2(am)$

→ no deviation (!?) from lowest order chiral perturbation theory

$$(am_P)^2 = B_M am , B_M = 4a \Sigma / f_X^2$$

(= GMOR Relation) ⇒ determine $\Sigma$

→ expect for quenched approximation:

$$m_\pi^2 = B_M am \left[ 1 - \delta (\ln(B_M am \Lambda_X^{-2})) \right] + B_M am + O(m^2)$$

→ use linear interpolation to match pseudoscalar masses
at $x_{ref} = (r_0 m_P)^2$
independence from $x_{\text{ref}}$

<table>
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<th>$\beta$</th>
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<th>$\hat{Z}_S$ (From $U_P$)</th>
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<td>5.0</td>
<td>1.00(5)</td>
<td>1.03(6)</td>
<td></td>
</tr>
</tbody>
</table>

$\Rightarrow$ comparison RGI condensate $\hat{\Sigma}$ from

FSS: $\hat{\Sigma} = 0.0138(16)(10) \text{GeV}^3$ \quad $\beta = 5.85$

slope: $\hat{\Sigma} = 0.0141(6)(11) \text{GeV}^3$ \quad $\beta = 5.85$

slope: $\hat{\Sigma} = 0.0144(6)(11) \text{GeV}^3$ \quad $\beta = 6.00$

$\Sigma_{\text{MS}}(2\text{GeV}) = (268 \pm 12\text{MeV})^3$

- eliminated $V \to \infty$ and $m \to 0$ limits
- stay with discretization errors
determination of $\hat{\Sigma}$ for Wilson fermions from lowest order chiral perturbation theory

$\Rightarrow$ continuum extrapolation


$\rightarrow$ scaling violations for overlap fermions seem to be small

$\rightarrow$ but large error, check in future simulations
Summary IV

- Chiral symmetry can be realized on the lattice

- allows to compute scalar condensate and test on spontaneous chiral symmetry breaking

- renormalization can be performed by utilizing results from Schrödinger functional calculations
  → matching condition on renormalization group invariant quantities

- example can be generalized to matrix elements
  - renormalization factors by Schrödinger functional
  - matrix elements in different lattice formulations