Structure Functions on the Lattice

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- Introduction
- Non-perturbative Renormalization
- Computation of Matrix Elements
- Non-perturbative Matching
- Summary

The John von Neumann-Institute of Computing (NIC)

coorporation between **DESY** and research centre Jülich

• NIC shall provide supercomputer resources





centre of Lattice gauge theory <u>Zeuthen</u>

- NIC shall maintain research groups
 - Elementary particle physics K.J.
 - Many particle physics P. Grassberger

general computational science <u>Jülich</u>

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

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

- In the Bjorken limit $(-q^2 = Q^2 \rightarrow \infty, x = Q^2/2(pq))$, 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"

$$W(Q^2) = \sum_{i,N} C_N^{(i)}(x^2) x^{\mu_1} \cdots x^{\mu_N} \mathcal{O}_{\mu_1 \cdots \mu_N}^{(i)}(0)$$

Moments of PDFs

• The moments of PDF are related to leading twist τ (τ =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

$$\sum_{f} f_f \propto \sigma \propto W \propto \mathcal{O}_{i}$$

these moments can be represented as expectation values of *local* operators

$$\langle P|O_{\mu_1...\mu_N}^{(i)}(0)|P\rangle = M_a^{(N-1)}(\mu)P_{\mu_1}\cdots P_{\mu_n}$$

Experimental situation → very precise maesurements: unpolarized structure functions in a wide kinematic regime

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



Global fits

general phenomenological ansatz

$$xf(x,Q_0^2) = Ax^{\alpha}(1-x)^{\beta}$$

 \Rightarrow fit to experimental data

 \Rightarrow 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



Uncertainties in global fits

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



see also: : A.D. Martin et.al. Alekhin, hep-ph/0211080attempt for direct comparison to lattice data:J. Bümlein and H. Böttcher, Nucl.Phys. B636 (2002) 225

Extraction of α_s

experimental evidence (SLAC):

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

 \rightarrow (Bjorken) scaling

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

- \rightarrow Parton model
- \rightarrow quarks

Extraction of α_s from scaling violation

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

$$\int_{0}^{1} x f(x, Q^{2}) \frac{dx}{x} = 3 \left[1 - \frac{\alpha_{s}(Q^{2})}{\pi} - a(n_{f}) \left(\frac{\alpha_{s}(Q^{2})}{\pi} \right)^{2} - b(n_{f}) \left(\frac{\alpha_{s}(Q^{2})}{\pi} \right)^{3} \right] + \Delta \mathrm{HT}$$

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

 \Rightarrow 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
- \Rightarrow lattice could help substantially





- \rightarrow important contribution from deep inelastic scattering
- \rightarrow important contribution from lattice calculations

Moments \leftrightarrow local operators

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

$$M_a^{(n)}(\mu) = \int_0^1 dx x^{n-1} f_a(x,\mu) \qquad n = 1, 2, \cdots$$

the reason is that the moments can be related to expectation values of *local operators* $\mathcal{O}_a^n \leftarrow$ suitable for the lattice

 $M_a^{(n)}(\boldsymbol{\mu}) = \langle \mathcal{O}_a^n \rangle$

 $\{p^{\mu_1}\cdots p^{\mu_n}\}_{\mathrm{TS}}\langle \mathcal{O}^n_a\rangle = \langle p|\bar{\psi}_a(x)\,\{\gamma^{\mu_1}iD^{\mu_2}\cdots iD^{\mu_n}\}_{\mathrm{TS}}\,\psi_a(x)|p\rangle$

- $\langle p|$ state vector of a hadron with momentum p
- D^{μ} covariant derivative (gauge invariance)
- TS means to take traceless symmetric part

Examples of Moments

unpolarized quark distributions:

$$\langle x^n \rangle \sim \langle | \overline{\psi} \gamma_{\{\mu} D_{\mu_1} \cdots D_{\mu_n\}} \psi | \rangle$$

spin-dependent structure function g_1 :

$$\langle (\Delta x)^n \rangle \sim \langle | \overline{\psi} \gamma_5 \gamma_{\{\mu} D_{\mu_1} \cdots D_{\mu_n\}} \psi | \rangle$$

spin-dependent structure function g_2 :

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

transversity structure function h_1 :

$$\langle (\delta x)^n \rangle \sim \langle | \overline{\psi} \gamma_5 \sigma_{\mu \{ \mu_1} D_{\mu_2} \cdots D_{\mu_n \}} \psi | \rangle$$

unpolarized gluon distribution

$$\langle x^n \rangle_g \sim \langle h \mid \sum_{\rho} \operatorname{Tr} \left(F_{\mu}{}^{\rho} D_{\mu_2} \cdots D_{\mu_n} F_{\rho\mu_1} \right) \mid h \rangle$$

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 μ_0

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

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

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

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 $\langle x \rangle_{SF}(\mu)$

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

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

$$f^{\mathbf{SF}}(\bar{g}^2(\boldsymbol{\mu})) = (\bar{g}^2(\boldsymbol{\mu}))^{-\gamma_0/2b_0} \exp\left\{-\int_0^{\bar{g}(\boldsymbol{\mu})} dg\left[\frac{\gamma(g)}{\beta(g)} - \frac{\gamma_0}{b_0g}\right]\right\}$$

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

knowing $O^{\rm ren}$ we can get "easily" the matrixelement in a desired scheme

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

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

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

 \Rightarrow make contact with analytical computations in perturbation theory!

How to get $O_{\text{INV}}^{\text{ren}}$?

$$O_{\rm INV}^{\rm ren} = O_{\rm SF}^{\rm ren}(\mu) \cdot f^{\rm SF}(\bar{g}^2(\mu)) = \frac{\langle \pi | \mathcal{O}_{\rm NS} | \pi \rangle}{Z^{\rm SF}(1/\mu)} \cdot f^{\rm SF}(\bar{g}^2(\mu))$$
$$= \frac{\langle \pi | \mathcal{O}_{\rm NS} | \pi \rangle}{Z^{\rm SF}(1/\mu_0)} \cdot \underbrace{\frac{Z^{\rm SF}(1/\mu_0)}{Z^{\rm SF}(1/\mu)}}_{\equiv \sigma(\mu/\mu_0, \bar{g}(\mu))} \cdot f^{\rm SF}(\bar{g}^2(\mu))$$
$$\equiv O_{\rm SF}^{\rm ren}(\mu_0) \underbrace{\sigma(\mu/\mu_0, \bar{g}(\mu)) \cdot f^{\rm SF}(\bar{g}^2(\mu))}_{\equiv \mathfrak{S}_{\rm INV}^{\rm UV}(\mu_0)}$$

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

 $O_{\mathrm{INV}}^{\mathrm{ren}} = O_{\mathrm{SF}}^{\mathrm{ren}}(\mu_0) \mathfrak{S}_{\mathrm{INV}}^{\mathrm{UV}}(\mu_0)$

Summary I

- Parton distribution functions are determined very precisely in experiments worldwide
- they provide important information about the spin structure of hadrons may give very precise value of α_2
- further our understanding of QCD or shed light on new physics
- important: also moments of parton distribution functions can be determined from experiment
 - accesible to lattice computations
 - need scale dependent renormalization
- most important theoretical quantity: renormalization group invariant matrix element

Z can be computed in practise 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. $x_0/L = 1/2$)

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

with some choice of the momentum ${\bf p}$ and $\Gamma=\gamma_2$

 ζ , $\overline{\zeta}$ are boundary quark fields at $x_0 = 0$ the desired value of \overline{Z} is then obtained by normalizing with $f_{\overline{Z}}^{\text{tree}}(x_0)$

$$\bar{Z}(L) = \frac{f_{\bar{Z}}(x_0)}{f_{\bar{Z}}^{\text{tree}}(x_0)} \bigg|_{x_0/L = \text{fixed}}$$



 \rightarrow need normalization of boundary fields

 $f_1 = -\frac{1}{L^6} \sum_{\mathbf{u}, \mathbf{v}, \mathbf{y}, \mathbf{z}} \frac{1}{3} \langle \bar{\zeta}'(\mathbf{u}) \Gamma_{\overline{4}}^1 \tau^3 \zeta'(\mathbf{v} \bar{\zeta}(\mathbf{y}) \Gamma_{\overline{4}}^1 \tau^3 \zeta(\mathbf{z}) \rangle$

definition of the normalization constant

space

$$Z(L) = \frac{\bar{Z}(L)}{\sqrt{f_1(L)}}$$

and we have the step scaling functions

$$\sigma_{\bar{Z}} = \frac{\bar{Z}(2L)}{\bar{Z}(L)}, \ \sigma_{f_1} = \frac{\sqrt{f_1}(2L)}{\sqrt{f_1}(L)}, \ \sigma_{Z} = \frac{Z(2L)}{Z(L)}$$

 \rightarrow note that so far the who discussion was in the continuum!

Excursion to the lattice

non-perturbative information from numerical simulations

 \rightarrow make $Z(\mu)$ dependend on the lattice spacing

 $Z(\boldsymbol{\mu}) = Z(\boldsymbol{\mu}, a)$

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 Σ_Z !): $\sigma_Z = \lim_{a\to 0} \Sigma_Z(a)|_{\mu^{-1}=L \text{ fixed}}$ how do we fix the scale?

 \rightarrow through the coupling constant $g = \bar{g}(\mu = 1/L)$ (computation of running coupling necessary prerequisite) continuum limit is reached through a matching procedure



 $\bar{g}^2(L)$ fixed

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 $\underline{m = 0} \leftarrow \text{Schrödinger functional boundary conditions}$

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 fixed

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

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

Strategy

- Compute (x)(β) between pion states in "infinite volume" with β(a) given by r₀ 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 μ) to small L (high μ)
- Continue with perturbative evolution to arrive at (scale and scheme independent) RGI matrix element
- Connection with experiment evolving in the $\overline{\mathrm{MS}}$ scheme

$\langle x angle_{RGI}$	<i>←</i>	$\langle x angle_{RGI}$
\downarrow		\uparrow
perturbative evolution		perturbative evolution
\downarrow		\uparrow
$\langle x angle_{\overline{\mathrm{MS}}}$ at $\mu=2~\mathrm{GeV}$		$\langle x angle_{SF}$ at $L=0.005$ fm
		↑ non- perturbative evolution
		↑ finite-volume
hadronic scheme	\longrightarrow	scheme $\langle x angle_{SF}$ at $L=0.7$ fm

Generalized boundary conditions in space

boundary conditions for fermions in spatial directions

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

implementation in the definition of the gauge covariant lattice derivatives:

$$\nabla_{\mu}\psi(x) = \frac{1}{a} \left[\lambda_{\mu}U(x,\mu)\psi(x+a\hat{\mu})-\psi(x)\right]$$
$$\nabla_{\mu}^{*}\psi(x) = \frac{1}{a} \left[\psi(x)-\lambda_{\mu}^{*}U(x-a\hat{\mu},\mu)\psi(x-a\hat{\mu})\right]$$
$$\lambda_{\mu} = e^{ia\theta_{\mu}/L}, \quad 0 \le \theta_{k} \le 2\pi, \quad \theta_{4} = 0,$$

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

$$\mathcal{O}_{12}(x) = \frac{1}{4}\bar{\psi}(x)\gamma_{\{1}\stackrel{\leftrightarrow}{D}_{2\}}\frac{1}{2}\tau^{3}\psi(x)$$
$$\mathcal{O}_{44}(x) = \frac{1}{2}\bar{\psi}(x)\left[\gamma_{4}\stackrel{\leftrightarrow}{D}_{4} - \frac{1}{3}\sum_{k=1}^{3}\gamma_{k}\stackrel{\leftrightarrow}{D}_{k}\right]\frac{\tau^{3}}{2}\psi(x) .$$

external momentum $\rightarrow \theta_k$

$$\theta \equiv \theta_1 \neq 0, \ \theta_2 = \theta_3 = 0$$

 θ appears in derivative and in propagators

Correlation functions at tree level



<u>Choice of θ </u>

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

Perturbation Theory

perturbative expansion

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

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

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

2-loop coefficient γ_1 in SF-scheme can be obtained by knowing 2-loop coefficient in a different scheme

$$\gamma_1 = \gamma_1^{\overline{\mathrm{MS}}} + 2b_0 \Delta Z_{\mathcal{O}}^{(1)} - \gamma_0 \mathcal{X}_{\mathrm{g}}^{(1)}$$

 $\Delta Z_{\mathcal{O}}^{(1)}$ 1-loop difference of renormalization constants $\mathcal{X}_{g}^{(1)}$ 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 \mathcal{O}_R^s renormalized in a certain scheme s is obtained by

 $\mathcal{O}_R^s = Z_{\mathcal{O}}^{s,reg} \mathcal{O}_b^{reg}$

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

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

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

 $\Delta Z_{\mathcal{O}}^{s' \leftarrow s}$ 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

 \rightarrow connect directly with the $\overline{\rm MS}$ scheme

Relating Schemes

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

$$\Delta Z_{\mathcal{O}}^{SF \leftarrow \overline{\mathrm{MS}}} = Z_{\mathcal{O}}^{SF,DR} / Z_{\mathcal{O}}^{\overline{\mathrm{MS}},DR}$$

However, $Z_{\mathcal{O}}^{SF,DR}$ not known \Rightarrow bridge via the MOM-scheme

the desired factor $\Delta Z_{\mathcal{O}}^{SF \leftarrow \overline{MS}}$ relating the SF to the \overline{MS} scheme are obtained by

$$\Delta Z_{\mathcal{O}}^{SF \leftarrow \overline{\mathrm{MS}}} = \Delta Z_{\mathcal{O}}^{SF \leftarrow MOM} \Delta Z_{\mathcal{O}}^{MOM \leftarrow \overline{\mathrm{MS}}}$$

two factors ΔZ are computed using different regularizations: $\Delta Z_{\mathcal{O}}^{SF \leftarrow MOM}$ computed on the lattice $\Delta Z_{\mathcal{O}}^{MOM \leftarrow \overline{\mathrm{MS}}}$ 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 $\Delta Z_{\mathcal{O}}^{(1)}$ and from this finally γ_1

Relating Schemes



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

 $\beta(g) \stackrel{g \to 0}{\sim} -g^3 \sum_{k=0}^{\infty} b_k g^{2k}, \gamma(g) \stackrel{g \to 0}{\sim} -g^2 \sum_{k=0}^{\infty} \gamma_k g^{2k}$ $C_F = (N_c^2 - 1)/2N_c \text{ and } N_c \text{ the number of colors})$ $b_0 = \left\{\frac{11}{3}N_c - \frac{2}{3}N_f\right\} (4\pi)^{-2}$ $\gamma_0 = \frac{16}{3}C_F (4\pi)^{-2}$ $b_1 = \left\{\frac{34}{3}N_c^2 - (\frac{13}{3}N_c - N_c^{-1})N_f\right\} (4\pi)^{-4}$

Any two mass independent renormalization schemes can be related by a scale change and a finite parameter renormalization of the form

 $\mu' = c\mu, \qquad c > 0$ $\bar{g}' = \bar{g}\sqrt{\mathcal{X}_{g}(\bar{g})}$ $Z' = Z[\Delta Z_{O}(\bar{g})],$ $\mathcal{X}_{g}(\bar{g}) \stackrel{\bar{g} \to 0}{\sim} 1 + \sum_{k=1}^{\infty} \mathcal{X}_{g}^{(k)} \bar{g}^{2k}.$ $\Delta Z_{O}(\bar{g}) \stackrel{\bar{g} \to 0}{\sim} 1 + \sum_{k=1}^{\infty} \Delta Z_{O}^{(k)} \bar{g}^{2k}.$

The invariance of a physical observable under such a change of parameters, gives a relation between the renormalization group functions, β and γ , in the 2 schemes. In particular we have

$$\gamma_{1} = \gamma_{1}^{\overline{\text{MS}}} + 2b_{0}\Delta Z_{O}^{(1)} - \gamma_{0}\mathcal{X}_{g}^{(1)}$$
$$\mathcal{X}_{g}^{(1)} = -\frac{1}{4\pi}(c_{1,0} + c_{1,1}N_{f})$$
$$c_{1,0} = 1.25563(4), \qquad c_{1,1} = 0.039863(2)$$

Anomalous dimensions

θ	$\gamma_1^A(heta)$	$\gamma^B_1(heta)_{2,b}$	$\gamma_1^A(heta)/\gamma_0$	$\gamma_1^B(heta)/\gamma_0$
0.1	0.06584(1)	0.06551(1)	1.4621(6)	1.4548(3)
0.4	0.06083(1)	0.05669(1)	1.3509(6)	1.2590(2)
0.7	0.05196(1)	0.04135(1)	1.1539(6)	0.9182(2)
1.0	0.04211(1)	0.02482(1)	0.9352(6)	0.5512(2)
1.3	0.03313(1)	0.01029(1)	0.7357(6)	0.2286(2)
1.6	0.02561(1)	-0.00139(1)	0.5687(6)	-0.0308(3)
1.9	0.01951(1)	-0.01051(1)	0.4332(6)	-0.2334(3)
2.2	0.01449(1)	-0.01775(1)	0.3217(6)	-0.3943(3)
2.5	0.01019(1)	-0.02375(1)	0.2263(6)	-0.5273(3)
2.8	0.00627(3)	-0.02903(3)	0.1392(6)	-0.6446(6)
3.1	0.00231(3)	-0.03412(3)	0.0512(6)	-0.7578(6)

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 $k(0; x_4/L, \theta) = -\gamma_0 \ln(2)$



 $\delta_{\mathbf{k}}(a/L; x_4/L, \theta) = \frac{k(a/L; x_4/L, \theta) - k(0)}{k(0)}$

Signal to Noise Ratio





Cutoff effects in Step Scaling Function

Start simulation with pure Wilson fermions (and Wilson plaquette action)



 $\theta = 0$ \mathcal{O}_{12} operator



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

$$\mathcal{O}_{\text{impr}} = c_{1} \bar{\psi} \gamma_{\mu} D_{\nu} \psi + c_{2} \bar{\psi} \sigma_{\mu\nu} F_{\mu\nu} + c_{3} \bar{\psi} \{ D_{\mu}, D_{\nu} \} + c_{4} \partial_{\lambda} \left(\bar{\psi} \sigma_{\mu\lambda} D_{\nu} \right)$$

 \Rightarrow complicated operator and difficult to determine the coefficients c_1, \cdots, c_4 non-perturbatively

- \rightarrow attempt to first only improve the action
- \rightarrow provides a check on the continuum extrapolation of σ



· · · pure Wilson

— O(a) improved Wilson σ_{f_1} for improved Wilson no cutoff effects — expected compatible continuum values

a/L



pure Wilson
 O(a) improved Wilson
 check on continuum
 extrapolation



parametrization $\sigma_{Z_{12}} = 1 - \gamma_0 \ln(2) g_0^2 + c_1 g_0^4 + c_2 g_0^6$

Renormalization Group Invariant Step Scaling Function

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

need step scaling function in steps of two \Rightarrow interpolation in g_0 be careful with error propagation:

$$(\Delta\sigma_{Z_{\mathcal{O}}}) = \sqrt{\frac{\partial\sigma_{Z_{\mathcal{O}}}}{\partial c_1}^2} (\Delta c_1)^2 + \frac{\partial\sigma_{Z_{\mathcal{O}}}}{\partial c_2}^2 (\Delta c_2)^2 + 2\frac{\partial\sigma_{Z_{\mathcal{O}}}}{\partial c_1} \cdot \frac{\partial\sigma_{Z_{\mathcal{O}}}}{\partial c_2} \cdot \operatorname{cov}_{12} + \frac{\partial\sigma_{Z_{\mathcal{O}}}}{\partial \bar{g}^2} \Delta \bar{g}^2$$

Renormalization Group Invariant Step Scaling Function



 $\mathfrak{S}_{\mathrm{INV},\mathcal{O}_{12}}^{UV,SF}(\mu_0) = 0.242(8), \ \mathfrak{S}_{\mathrm{INV},\mathcal{O}_{44}}^{UV,SF}(\mu_0) = 0.221(9) \ .$

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

$$\lim_{a \to 0} \left. \frac{\langle \pi | \mathcal{O}_2 | \pi \rangle}{Z_{O_2}(L_0)} \right|_{m_q = 0}$$

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

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

 \Rightarrow fine adjustment of $\beta=6/g_0^2$



use SF to compute the matrix element



keep plateau length for extracting the

matrix element fixed to be 1 fm

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

$$\mathcal{O}_{44}(x) = \frac{1}{2}\bar{\psi}(x) \left[\gamma_4 \stackrel{\leftrightarrow}{D}_4 - \frac{1}{3}\sum_{k=1}^3 \gamma_k \stackrel{\leftrightarrow}{D}_k \right] \psi(x)$$
$$\mathbf{S} = \frac{a^6}{L^3} \sum_{\mathbf{y},\mathbf{z}} \bar{\zeta}(\mathbf{y}) \gamma_5 \tau^+ \zeta(\mathbf{z}) , \quad \mathbf{S}' = \frac{a^6}{L^3} \sum_{\mathbf{u},\mathbf{w}} \bar{\zeta}'(\mathbf{u}) \gamma_5 \tau^- \zeta'(\mathbf{w})$$

Consider then the correlation functions

$$f_{44}(x_0) = \langle \mathbf{S}\mathcal{O}_{44}(x)\mathbf{S}' \rangle$$
$$f_1 = -\frac{1}{2} \langle \mathbf{S}\mathbf{S}' \rangle$$

quantum mechanical interpretation

$$f_{44}(x_0) = \mathcal{Z}^{-1} \langle i_\pi | e^{-(T-x_0)\mathbf{H}} \mathbf{P} \mathcal{O}_{44}(x) e^{-x_0\mathbf{H}} \mathbf{P} | i_\pi \rangle , \quad f_1 = \mathcal{Z}^{-1} \frac{1}{2} \langle i_\pi | e^{-T\mathbf{H}} \mathbf{P} | i_\pi \rangle$$

P projector on gauge invariant states

Inserting a complete set of eigenstates of the hamiltonian

correlation function

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

pion gap: $\Delta r_0 \approx 3.2$ $0^{++}mass: m_G r_0 \approx 4.3$

• matrix element

$$f_{44}(x_0) \simeq \rho^2 \langle 0, \pi | \mathcal{O}_{44}(x) | 0, \pi \rangle e^{-m_\pi T} \{ 1 + \eta_{\mathcal{O}_{44}}^\pi e^{-x_0 \Delta} + \eta_{\mathcal{O}_{44}}^\pi e^{-(T-x_0)\Delta} \}$$

bounday 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,

$$m_{eff}(x_0) \approx m_{\pi} + \Delta \eta_A^{\pi} e^{-\Delta x_0} - m_G \eta_A^0 e^{-m_G (T-x_0)}$$
$$\langle x \rangle(x_0) \approx \langle x \rangle \left\{ 1 + \eta_M^{\pi} \left(e^{-\Delta x_0} + e^{-\Delta (T-x_0)} \right) \right\}$$

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

 \Rightarrow choose value of x_0 large enough to read off effective masses and plateaus for matrix element



 \rightarrow corrections consistent with estimate of higher state contributions

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 fm $\leq x_0 \leq$ 2.4 fm $m_{
m eff}$ 1.3 fm $\leq x_0 \leq$ 2.2 fm matrix element



Finite volume effects for pion mass: $m_{\pi}(L) = c_0 + c_1/L^{3/2} \exp(-c_2 L)$

 \rightarrow no effects for lattice sizes larger than $L\approx 1.2$ fm and $T\approx 2.8$ fm

Finite volume effects for the pion matrix element:



power law $\langle x \rangle(L) = c_0 + c_1/L^{c_2}$

exponential $\langle x \rangle(L) = c_0 + c_1/L^{3/2} \exp(-c_2 L)$

 \rightarrow large volumes $L\approx 1.9$ fm and $T\approx 3.3$ fm needed

 \Rightarrow warning for nucleon matrix elements



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)



note the operator $\mathcal{O}_{12}(x) = \bar{\psi}(x)\gamma_{\{1} \stackrel{\leftrightarrow}{D}_{2\}} \frac{1}{2}\tau^3\psi(x)$ needs an external momentum to saturate indices \Rightarrow very noisy

continuum limit of renormalized matrix element

$$\langle x \rangle_{\mathrm{SF}}(\mu_0) = \lim_{a \to 0} \left. \frac{\langle \pi | \mathcal{O}_2 | \pi \rangle}{Z_{O_2}(L_0)} \right|_{m_q = 0}$$

• use two action method to check for universal continuum limit



linear chiral extrapolation

$$\langle x \rangle_{\rm SF}(\mu_0) = \\ \lim_{a \to 0} \lim_{\rm chiral} \frac{\langle \pi | \mathcal{O}_{\rm NS}^{n=2} | \pi \rangle}{Z^{\rm SF}(1/\mu_0)} = \\ 0.870(33)$$

renormalization group invariant matrix element



renormalization group invariant matrix element



- NLO analysis of Drell-Yan and prompt photon πN data (NA10 and E615 collaboration)
 SMRS, PRD 45 (1992) 2349
 GRS, Eur.Phys.J.C10 (1999) 313
- lattice result evolved in perturbation theory using the RGI matrix element

Summary III

- Schrödinger Functional is <u>also</u> well suited to determine *matrix elements*
- determine continuum matrix element at a small scale μ_0
- determination of renormalization group invariant matrix element
 - relation to $\overline{\mathrm{MS}}$ 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

Quantumchromodynamics

massless QCD has chiral symmetry

$$\psi \to e^{i\theta\gamma_5}\psi, \quad \bar{\psi} \to \bar{\psi}e^{i\theta\gamma_5}\psi$$

or, equivalently, $\gamma_5 D_{\text{cont}} + D_{\text{cont}} \gamma_5 = 0$, D_{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

(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 γ_5 at all non-zero distances

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

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

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

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 ${\cal D}$ which satisfies the Ginsparg-Wilson relation, the action

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

is invariant under the transformations

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

 \Rightarrow have a notion of chiral symmetry on the lattice

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

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_{\rm ov} is local, \|D_{\rm ov}\Phi\| \propto e^{-\gamma/a}
(Hernandèz, Lüscher, K.J.)
```

- if plaquette is bounded: $||1 U_P|| < 1/30$ (analytical proof)
- locality also demosntrated numerically when bound not satisfied

 \Rightarrow

- chiral symmetric
- local

lattice QCD \rightarrow non-perturbative definition of QCD ($a \rightarrow 0$)

practical application: spontaneous chiral symmetry breaking in QCD

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

- ⇒ 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 enviroment to test this basic assumption and an operator satisfying the Ginsparg-Wilson relation provides the neccessary tool to perform this test in practise 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 Vin quenched chiral perturbation theory has been worked out (Damgaard, Osborn, Toublan, Verbaaschoot)

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

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

for $m \rightarrow 0$ approximate formulae are obtained

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

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

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



⇒ find strong evidence for spontaneous chiral symmetry breaking in QCD!

Systematic uncertainties of $\langle \bar{\psi}\psi \rangle$:

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

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

- 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 μ dependent renormalization factor
- ii) only one value of the lattice spacing \rightarrow need continuum extrapolation
- iii) quenched approximation \rightarrow include effects of dynamical quarks

renormalization factor $Z(\mu)$

in principle: need a box covering all energy scales

```
a \ll \underbrace{0.001 \text{fm}}_{M_W} - \underbrace{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
- → 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

 \rightarrow fix *physical* situation: choice $(r_0 M_P)^2 = x_{\rm ref}$ fixed

 \Rightarrow match *renormalizion group invariant* (RGI) quantities

- RGI quark mass M = Z_M(g₀)m(g₀)
 m current quark mass
 (=bare quark mass for overlap fermions)
- RGI matrix element 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)

$$Z_{M}^{ov}(g_{0})m^{ov}(g_{0}) = Z_{M}^{w}(g_{0}^{'})m^{w}(g_{0}^{'})\Big|_{x_{\text{ref}}}$$

$$Z_{P}^{ov}(g_{0})G_{P}^{ov}(g_{0}) = Z_{P}^{w}(g_{0}^{'})\frac{\bar{m}}{M}G_{P}^{w}(g_{0}^{'})\Big|_{x_{\text{ref}}}$$

why is this helpful for renormalizing $\langle \bar{\Psi}\Psi
angle ?$

 \rightarrow for chiral invariant formulations

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

putting in a physical scale

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

- $r_0 = 0.49 \mathrm{fm}$ 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

$$U_{M} = \lim_{g'_{0} \to 0} \left\{ Z_{m}^{wil}(g'_{0})(r_{0}m_{wil})(g'_{0}) \right\} \Big|_{x_{ref}}$$

similar a U_P for the pseudoscalar matrix element can be computed

$$U_P = \lim_{g'_0 \to 0} \left\{ Z_P^w(g'_0) \frac{\bar{m}^{\rm SF}}{M} \times (1 + ab_P m_q) (r_0^2 G_P^w)(g'_0) \right\} \Big|_{x_{ref}}$$

b_P improvement coefficient

- \Rightarrow only remaining lattice artefacts from overlap fermions
- \Rightarrow check on scaling behaviour fermions

 \Rightarrow knowing $Z_{\rm m}^{\rm ov}(g_0)$ and $\Sigma_{\rm bare}(g_0)$

define a renormalization group invariant scalar condensate

$$\hat{\Sigma} = \frac{1}{Z_{\rm m}^{\rm ov}(\boldsymbol{g_0})} \Sigma_{\rm bare}(\boldsymbol{g_0})$$

knowing $\hat{\Sigma}$

- \rightarrow 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

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

 \Rightarrow obtain a fully renormalized quark condensate

Pseudoscalar mass for overlap and Wilson fermions



- $\rightarrow \text{ expect for quenched approximation:} \\ m_{\pi}^2 = B_M am \left[1 \delta(\ln(B_M am \Lambda_{\chi}^{-2})) \right] + B_M am + O(m^2)$
- $\rightarrow\,$ use linear interpolation to match pseudoscalar masses at $x_{\rm ref}=(r_0m_P)^2$

independence from x_{ref}

			From U_M	From U_P
	eta	x_{ref}	\hat{Z}_S	\hat{Z}_S
·	5.85	1.5736	1.05(25)	1.03(15)
		3.0	1.04(8)	1.04(8)
		5.0	0.99(4)	0.99(6)
	6.00	1.5736	0.98(17)	1.05(14)
		3.0	1.03(8)	1.07(8)
		5.0	1.00(5)	1.03(6)

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

FSS: $\hat{\Sigma} = 0.0138(16)(10) \text{GeV}^3$ $\beta = 5.85$ slope: $\hat{\Sigma} = 0.0141(6)(11) \text{GeV}^3$ $\beta = 5.85$ slope: $\hat{\Sigma} = 0.0144(6)(11) \text{GeV}^3$ $\beta = 6.00$

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

- 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



Giusti et.al., hep-lat/0108007 and hep-lat/0110184; Gisuti et.al., Nucl.Phys. B538 (1999) 249; Gupta et.al., Phys.Rev.D55 (1997) 7203

- \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
 - \rightarrow 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