# Non-perturbative Renormalization 

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## Nonperturbative Renormalization

First consider just the renormalization of the coupling, set

$$
m_{i}=0
$$

## Properties of a renormalised coupling

a finite: $g=f\left(g_{0}, \mu a\right)$, such that $\left.\lim _{a \rightarrow 0} G_{0}\left(q a, g_{0}\right)\right|_{g}$ exists
b gauge invariant (physical)
most natural

$$
\begin{array}{ll} 
& G_{0}=G_{0}\left(q a, g_{0}\right) \\
\rightarrow \quad & G_{\mathrm{R}}=G_{\mathrm{R}}\left(q / m_{\text {proton }}, q a\right), \quad a m_{\text {proton }}=f\left(g_{0}\right) \\
& G_{\mathrm{R}}^{\text {cont }}=G_{\mathrm{R}}\left(q / m_{\text {proton }}, 0\right)
\end{array}
$$

"hadronic scheme"

- but we want a coupling, i.e. the relation to the $\Lambda$ - parameter, the relation to perturbative QCD


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C

$$
\begin{aligned}
& g_{\mathrm{NP}}^{2} \stackrel{g_{\mathrm{lat}} \rightarrow 0}{\sim} \quad g_{\mathrm{lat}}^{2} \chi_{g}^{\mathrm{NP}, \text { lat }}\left(g_{\mathrm{lat}}\right) \\
& \chi_{g}^{x, y}(g)= 1+\chi_{g, 1}^{x, y} g^{2}+\ldots \\
& \uparrow \\
& \\
& \text { convention, good idea }
\end{aligned}
$$

d It depends on a single scale $\mu \quad \rightarrow$ RGE! For $\mu \rightarrow \infty$ it is purely short distance

## Nonperturbative Renormalization

## Generic definition of a renormalized coupling

Take $G_{0}\left(\mu a, g_{0}\right)$ dimensionless (in the massless theory) satisfying a,b,d.
$G_{0}$ has a regular PT

$$
\begin{align*}
G_{0}\left(q a, g_{0}\right)= & G_{0}^{(0)}(q a)+G_{0}^{(1)}(q a) g_{0}^{2}+G_{0}^{(2)}(q a) g_{0}^{4}+\ldots \\
\text { lat scheme: } & g_{0}^{2}=g_{\mathrm{lat}}^{2}+2 b_{0} \ln (a \mu) g_{\mathrm{lat}}^{4}+\ldots \\
\rightarrow \quad G_{0}=G_{\mathrm{R}}= & G_{\mathrm{R}}^{(0)}(q a)+G_{\mathrm{R}}^{(1)}(q a) g_{\mathrm{lat}}^{2}+G_{\mathrm{R}}^{(2)}(q / \mu, q a) g_{\mathrm{lat}}^{4}+\ldots \\
i=0,1: \quad & G_{\mathrm{R}}^{(i)}(q a)=G_{0}^{(i)}(q a)=C^{(i)}+\mathrm{O}\left(a^{2} q^{2}\right)  \tag{*}\\
& G_{\mathrm{R}}^{(2)}(q / \mu, q a)=G_{0}^{(2)}(q a)+2 b_{0} \ln (a \mu) G_{0}^{(1)}(q a) \\
& =H(q a)+2 b_{0} \ln (\mu / q) G_{0}^{(1)}(q a)  \tag{*}\\
& H(q a)=C^{(2)}+\mathrm{O}\left(a^{2} q^{2}\right)
\end{align*}
$$

(*): the continuum limit exists

## Nonperturbative Renormalization

## Generic definition of a renormalized coupling

Set $\mu=q$ :

$$
\begin{aligned}
G_{0}\left(\mu a, g_{0}^{2}\right) & =G_{\mathrm{R}}^{(0)}(\mu a)+G_{\mathrm{R}}^{(1)}(\mu a) g_{\mathrm{lat}}^{2}(\mu)+G_{\mathrm{R}}^{(2)}(1, \mu a) g_{\mathrm{lat}}^{4}(\mu)+\ldots \\
& =G_{0}^{(0)}(\mu a)+G_{0}^{(1)}(\mu a) g_{\mathrm{lat}}^{2}(\mu)+\underbrace{G_{\mathrm{R}}^{(2)}(1, \mu a)}_{C^{(2)}+\mathrm{O}\left(a^{2} q^{2}\right)} g_{\mathrm{lat}}^{4}(\mu)+\ldots
\end{aligned}
$$

then

$$
\bar{g}_{G}^{2}(\mu) \equiv \frac{G_{0}\left(\mu a, g_{0}^{2}\right)-G_{0}^{(0)}(\mu a)}{G_{0}^{(1)}(\mu a)}
$$

satisfies a,b,c,d

## Nonperturbative Renormalization

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\end{aligned}
$$

then

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$$

satisfies a,b,c,d

## "physical" coupling

note

$$
\begin{aligned}
\bar{g}_{G}^{2}(\mu)= & 1 \times g_{\text {lat }}^{2}+\mathrm{O}\left(g_{\mathrm{lat}}^{4}\right) \\
& \uparrow \\
& \text { no } a^{2} \text { effects here }
\end{aligned}
$$

## Nonperturbative Renormalization

## Example 1

$Q \bar{Q}$ potential, force:

$$
\begin{aligned}
G_{0}\left(\mu a, g_{0}^{2}\right)= & r^{2} F_{\mathrm{impr}}(r), \quad \mu=1 / r
\end{aligned} \quad \mathrm{q} \quad \overline{\mathrm{q}} .
$$

def. of $F_{\text {impr }}$ later

$$
\rightarrow \quad \bar{g}_{\mathrm{qq}}^{2}(\mu)=\frac{4 \pi}{C_{F}} r^{2} F_{\mathrm{impr}}(r)
$$

[there is a little caveat with this ... not $100 \%$ short distance ... but ok]

## Nonperturbative Renormalization

## Example 2

Two-point function of multiplicatively renormalisable field

$$
G_{0}\left(\mu a, g_{0}^{2}\right)=\frac{\left\langle P^{r s}(x) P^{s r}(0)\right\rangle_{x=(0,0,0,1 / \mu)}}{\left\langle P^{r s}(x) P^{s r}(0)\right\rangle_{x=(0,0,0,2 / \mu)}}
$$



- Factors $Z_{\mathrm{P}}$ cancel
- Theoretically fine, but not really recommended (by me) in practise

$$
\left.\left\langle P^{r s}(x) P^{s r}(0)\right\rangle\right\rangle^{x \rightarrow 0} x^{-6}
$$

steep function, large $(a / x)^{n}$ effects

## Nonperturbative Renormalization

- case by case
- eg. (in principle)

$Z_{\mathrm{P}}^{2}\left(a \mu, g_{0}\right)\left\langle P^{r s}(x) P^{s r}(0)\right\rangle_{x=(0,0,0,1 / \mu)}=\left\langle P^{r s}(x) P^{s r}(0)\right\rangle_{x=(0,0,0,1 / \mu), g_{0}=0}$
this defines $Z_{\mathrm{P}}\left(a \mu, g_{0}\right)$
- many correlation functions of $P^{r s}$ can be used, as long as they are sufficiently short distance dominated
- but be careful with integrals, e.g.

$$
\int \mathrm{d}^{4} x\left\langle P^{r s}(x) P^{s r}(0)\right\rangle
$$

does not exist, since $\left\langle P^{r s}(x) P^{s r}(0)\right\rangle \stackrel{x \rightarrow 0}{\sim} x^{-6}$

## Nonperturbative Renormalization

## RI-MOM: the principle idea [ ©. Martinemli, c. P. Pitori, C. T. Sachrajida, M. Testa \& A. Vladikas 1995]

drop gauge invariance requirement (b): fix a gauge (e.g. Landau gauge) numerical evidence that this can be done non-perturbatively
then

$$
\begin{aligned}
& S(p)=a^{8} \sum_{x_{1}, x_{2}} \exp \left(-i p\left(x_{1}-x_{2}\right)\right)\left\langle\psi_{r}\left(x_{1}\right) \bar{\psi}_{r}\left(x_{2}\right)\right\rangle \\
& G_{P}\left(p_{1}, p_{2}\right)=a^{8} \sum_{x_{1}, x_{2}} \exp \left(-i p_{1} x_{1}+i p_{2} x_{2}\right)\left\langle\psi_{r}\left(x_{1}\right) P^{r s}(0) \bar{\psi}_{s}\left(x_{2}\right)\right\rangle \\
& \Lambda_{P}\left(p_{1}, p_{2}\right)=S^{-1}\left(p_{1}\right) G_{P}\left(p_{1}, p_{2}\right) S^{-1}\left(p_{2}\right) \\
& \Gamma_{P}\left(p_{1}, p_{2}\right)=\frac{1}{12} \operatorname{Tr}\left[\gamma_{5} \Lambda_{P}(p, p)\right], \quad \Gamma_{V}\left(p_{1}, p_{2}\right)=\ldots
\end{aligned}
$$

Define $\Gamma_{V}(p)$ similarly from the conserved vector current, then

$$
Z_{\mathrm{P}} \Gamma_{P}\left(p_{1}, p_{2}\right) / \Gamma_{V}\left(p_{1}, p_{2}\right)=\left[\Gamma_{P}\left(p_{1}, p_{2}\right) / \Gamma_{V}\left(p_{1}, p_{2}\right)\right]_{g_{0}=0}
$$

defines $Z_{\mathrm{P}}(\mu)$ [or use a similar condition for the quark propagator to define the quark field renormalization constant and divide it out in $\Lambda_{P}$ ]
symmetric point $p^{2}=p_{1}^{2}=p_{2}^{2}=\left(p_{1}-p_{2}\right)^{2}=\mu^{2}$
$\rightarrow$ short distance dominated "RI-sMOM"
[C. Sturm, Y. Aoki, N. H. Christ, T. Izubuchi, C. T. C. Sachrajda \& A. Soni, ARXIV:0901.2599 ]

## Scale Problem

( $\alpha_{\mathrm{qq}}$ as an example)
We need to reach large $\mu$ where perturbation theory is reliable to be able to use the perturbative relation (perturbative $\beta$-function) in

$$
\frac{\Lambda}{\mu}=\varphi_{g}(g(\mu))
$$




Let us see this in more detail

## Scales, lattices

- L/a=32, ... 192, L=2fm (big enough in YM), open BC (no topology freezing)



## Strategy to get to small r (see also arXiv:1711.01860)

- basic scale from $t_{0}$ :

$$
\alpha_{\mathrm{qq}}\left(\mu, a^{2} \mu^{2}\right), \quad \mu=1 / r=\left(x \sqrt{8 t_{0}}\right)^{-1}
$$

on ensembles with $a>0.02 \mathrm{fm}$

- Then step scaling functions

$$
\Sigma(u, a / r)=\left.\bar{g}_{\mathrm{qq}}^{2}(s r)\right|_{\bar{g}_{\mathrm{qq}}^{2}(r)=u}
$$

with $s=3 / 4$ including $a=\{1.0,1.4,2.0\} \times 10^{-2} \mathrm{fm}$

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on ensembles with $a>0.02 \mathrm{fm}$

$$
0.25 \leq x \leq 0.4
$$

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## Continuum limits

- Large r region ( $r>0.1 \mathrm{fm}$ )


- Gradient flow: log-corrections to $a^{2}$ not yet known.


## Force


perturbative prediction with known $\Lambda$

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- perturbative prediction with known $\Lambda$
- Qualitative contact to PT is made

- perturbative prediction with known $\Lambda$
- Qualitative contact to PT is made
- But is this safe to determine the $\Lambda$-parameter?


## Lambda parameter from $\alpha_{q q}$

$$
\Lambda / \mu=\varphi_{g}(g)==\left(b_{0} g^{2}\right)^{-b_{1} /\left(2 b_{0}^{2}\right)} \mathrm{e}^{-1 /\left(2 b_{0} g^{2}\right)} \exp \left\{-\int_{0}^{g} \mathrm{~d} x\left[\frac{1}{\beta(x)}+\frac{1}{b_{0} x^{3}}-\frac{b_{1}}{b_{0}^{2} x}\right]\right\}
$$

approximations：

$$
\begin{aligned}
& \left.\frac{\Lambda}{\mu}\right|_{n-\text { loop }} ^{\text {eff }}=\left(b_{0} g^{2}\right)^{-b_{1} /\left(2 b_{0}^{2}\right)} \mathrm{e}^{-1 /\left(2 b_{0} g^{2}\right)} \exp \left\{-\int_{0}^{g} \mathrm{~d} x\left[\frac{1}{\beta_{n-l o p}(x)}+\frac{1}{b_{0} x^{3}}-\frac{b_{1}}{b_{0}^{2} x}\right]\right\} \\
& \left.\frac{\Lambda}{\mu}\right|_{2-\text {-loop }} ^{\text {eff }}=\frac{\Lambda}{\mu}+\mathrm{O}\left(\alpha_{\mathrm{qq}}\right) \\
& \left.\frac{\Lambda}{\mu}\right|_{n-\text { loop }} ^{\text {eff }}=\frac{\Lambda}{\mu}+\mathrm{O}\left(\alpha_{\mathrm{qq}}^{n-1}\right)
\end{aligned}
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## Lambda parameter from $\alpha_{\mathrm{qq}}$

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A specialty of qq-coupling: at high orders there are infrared divergencies, need to be resummed, produce $\log (\boldsymbol{\alpha})$ terms $\rightarrow>$

## Lambda parameter from $\alpha_{\mathrm{qq}}$

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$$

$$
\left.\frac{\Lambda}{\mu}\right|_{2-\mathrm{loop}} ^{\mathrm{eff}}=\frac{\Lambda}{\mu}+\mathrm{O}\left(\alpha_{\mathrm{qq}}\right)
$$

computed from
Peter 97; Schröder 99

$$
\left.\frac{\Lambda}{\mu}\right|_{n-\mathrm{loop}} ^{\mathrm{eff}}=\frac{\Lambda}{\mu}+\mathrm{O}\left(\alpha_{\mathrm{qq}}^{n-1}\right)
$$

Anzai, Kiyo, Sumino, 10
Smirnov, Smirnov, Steinhauser, 10
Brambilla, Pineda, Soto, Vairo, 99
Kniehl, Penin, 99
Brambilla, Garcia i Tormo, Soto, Vairo, 07, 09

A specialty of qq-coupling: at high orders there are infrared divergencies, need to be resummed, produce $\log (\boldsymbol{\alpha})$ terms $\rightarrow>$

$$
\begin{aligned}
\beta_{3 \text {-loop }}(g)=-g^{3}[ & \left.b_{0}+b_{1} g^{2}+b_{2} g^{4}\right] \\
\text { 4-loop: } & +b_{3} g^{6}+b_{3 \mathrm{~L}} g^{6} \log (\alpha) \\
\text { 4-loop LL: } & +b_{4 \mathrm{~L}} g^{8} \log (\alpha)+b_{4 \mathrm{LL}} g^{8}[\log (\alpha)]^{2}
\end{aligned}
$$

## Results (from 2-stage continuum limit, standard derivative)



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## Results (from 2-stage continuum limit, standard derivative)



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## Results (from 2-stage continuum limit, standard derivative)



## Scale Problem

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```
( \(\alpha_{\mathrm{qq}}\) as an example)
```



$$
\begin{array}{ccccc}
L \\
\text { box size }
\end{array}>\begin{array}{ccc}
\frac{1}{0.2 \mathrm{GeV}} & \gg \hat{\uparrow} & \sim \frac{1}{10 \mathrm{GeV}}
\end{array} \begin{gathered}
\uparrow \\
\\
\end{gathered}
$$

## Scale Problem




$$
\text { Solution: } L=1 / \mu \longrightarrow \text { left with }
$$

$$
L / a \gg 1 \quad \text { Liseser, Wess, wotf] }
$$

Finite size effect as a physical observable; finite size scaling!

## Strategy

finite volume coupling $\alpha_{\mathrm{SF}}(\mu), \mu=1 / L$ defined at zero quark mass

$$
\begin{array}{cc}
L_{\max }=\text { const. } / m_{\mathrm{prot}}=\mathrm{O}\left(\frac{1}{2} \mathrm{fm}\right): & \alpha_{\mathrm{SF}}\left(\mu=1 / L_{\max }\right) \\
\downarrow \\
\text { always } a / L \ll 1 & \alpha_{\mathrm{SF}}\left(\mu=2 / L_{\max }\right) \\
\downarrow \\
\bullet \\
\bullet \\
\bullet \\
& \downarrow \\
& \alpha_{\mathrm{SF}}\left(\mu=2^{n} / L_{\max }=1 / L_{\min }\right) \\
& \mathrm{PT}: \quad \downarrow \\
\Lambda_{\mathrm{SF}} L_{\max }=\#
\end{array}
$$

Result is a value for $\Lambda_{\mathrm{SF}} / m_{\text {prot }}=\#$

## The step scaling function

We leave the discussion of a finite volume coupling for later. Discuss first the

Step scaling function

- It is a discrete $\beta$ function:

$$
\sigma\left(s, \bar{g}^{2}(L)\right)=\bar{g}^{2}(s L) \quad \text { mostly } s=2
$$

## The step scaling function

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- It is a discrete $\beta$ function:

$$
\sigma\left(s, \bar{g}^{2}(L)\right)=\bar{g}^{2}(s L) \quad \text { mostly } s=2
$$

- determines the non-perturbative running:

$$
\begin{aligned}
u_{0} & =\bar{g}^{2}\left(L_{\max }\right) \\
& \downarrow \\
\sigma\left(2, u_{k+1}\right) & =u_{k} \\
& \downarrow \\
u_{k} & =\bar{g}^{2}\left(2^{-k} L_{\max }\right)
\end{aligned}
$$



## The step scaling function

On the lattice:
additional dependence on the resolution $a / L$ $g_{0}$ fixed, $L / a$ fixed:


$\Sigma(2, \mathrm{u}, 1 / 6)$


## continuum limit:

$$
\Sigma(s, u, a / L)=\sigma(s, u)+\mathrm{O}(a / L)
$$

in the following always $s=2$

$$
\overline{\mathrm{g}}^{2}=\mathrm{u}
$$


everywhere: $m=0$ (PCAC mass defined in $(L / a)^{4}$ lattice)

## The step scaling function



| $L / a$ | $\beta$ | $\kappa$ | $\bar{g}^{2}$ | $d \bar{g}^{2}$ | $m$ | $d m$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $u=1.1814$ |  |  |  |  |  |  |
| 4 | 8.2373 | 0.1327957 | 1.1814 | 0.0005 | 0.00100 | 0.00011 |
| 5 | 8.3900 | 0.1325800 | 1.1807 | 0.0012 | -0.00018 | 0.00009 |
| 6 | 8.5000 | 0.1325094 | 1.1814 | 0.0015 | -0.00036 | 0.00003 |
| 8 | 8.7223 | 0.1322907 | 1.1818 | 0.0029 | -0.00115 | 0.00004 |
| 8 | 8.2373 | 0.1327957 | 1.3154 | 0.0055 | 0.00020 | 0.00005 |
| 10 | 8.3900 | 0.1325800 | 1.3287 | 0.0059 | 0.00097 | 0.00007 |
| 12 | 8.5000 | 0.1325094 | 1.3253 | 0.0067 | -0.00102 | 0.00002 |
| 16 | 8.7223 | 0.1322907 | 1.3347 | 0.0061 | -0.00194 | 0.00002 |
| $L / a$ |  |  | $\Sigma(1.1814, a / L)$ | $\delta \Sigma$ |  |  |
| 4 |  |  | 1.3154 | 0.0055 |  |  |
| 5 |  |  | 1.3296 | 0.0061 |  |  |
| 6 |  |  | 1.3253 | 0.0070 |  |  |
| 8 |  |  | 1.3342 | 0.0071 |  |  |

- tune $\kappa, g_{0}$ to have desired $m \approx 0$, fixed $\bar{g}^{2}(L)$
- propagate errors from $\bar{g}^{2}(L)$, shift mean values if necessary
$\longrightarrow \Sigma, \delta \Sigma$


## Example continuum extrapolation of step scaling functions

Continuum extrapolations of $\sigma(u)=\Sigma(u, 0), N_{\mathrm{f}}=3$


## The $\beta$-function from the step scaling function

$$
\int_{g(\mu)}^{\sigma(g(\mu))} \frac{-1}{\beta(x)} \mathrm{d} x=\log (2)
$$



## The $\beta$-function from the step scaling function

$$
\int_{\sqrt{u}}^{\sqrt{\sigma(u)}} \frac{-1}{\beta(x)} \mathrm{d} x=\log (2)
$$



## The $\beta$-function from the step scaling function

$$
\int_{\sqrt{u}}^{\sqrt{\sigma(u)}} \frac{-1}{\beta(x)} \mathrm{d} x=\log (2)
$$

- smooth fit function for $\beta(\mathbf{x})$



## Non-perturbative $\beta$-functions for $\mathrm{N}_{\mathrm{f}}=3$ QCD



## Non-perturbative $\beta$-functions for $\mathrm{N}_{\mathrm{f}}=3$ QCD



## Non-perturbative $\beta$-functions for $\mathrm{N}_{\mathrm{f}}=3$ QCD



## Overall strategy

$\alpha_{s}(\mu)$
$f_{\mathrm{K}}: K \rightarrow \ell \nu$ $f_{\pi}: \pi \rightarrow \ell \nu$
hadronic (low energy) scale


## Overall strategy

$\alpha_{s}(\mu)$
$f_{K}: K \rightarrow \ell \nu$
$f_{\pi}: \mathbb{T} \rightarrow \ell \nu$$\quad$ hadronic (low energy) scale


## Overall strategy

$$
\begin{gathered}
\alpha_{\mathrm{s}}(\mu) \mid \\
f_{\mathrm{K}}: K \rightarrow \ell \nu \\
f_{\pi}: \pi \rightarrow \ell \nu
\end{gathered}
$$



## Overall strategy



## Overall strategy



## Overall strategy

$\alpha_{s}(\mu) \mid$ 1. hadronic (low energy) scale


## 1. Determination of hadronic scale: CLS Ensembles

- CLS Ensembles
- Large volume, large scale simulations, with theoretically well founded improved Wilson action
- coordinated between

CERN<br>MADRID<br>MAINZ<br>MILANO + ROMA<br>REGENSBURG<br>DESY, Standort ZEUTHEN

coordinated by S. Schaefer, Data management H. Simma

## 1. Determination of hadronic scale: CLS Ensembles

## - finite L ...

simulated at common $\mathrm{g}_{0} \Leftrightarrow$ common lattice spacing a


## Adding in c, b, t - quarks by perturbation theory (see later)

add charm
$\alpha_{s}(\mu)$
$0.4-$
$0.35-$
$0.3-$
$0.25-$
$0.2-$
$0.15-$
0.1
0.05
0
0
10

Weinberg (80),
Bernreuther\&Wetzel (82),

Chetyrkin, Kühn \& Sturm;
Schröder, Steinhauser (06)
5-loop $\beta$-fct:
Baikov, Chetyrkin, Kühn; Luthe, Maier, Marquard,
Schrl"oder (16)
add beauty

- 4-loop PT available
- adding fermion loops, "only"
- perturbative uncertainties are tiny

$$
\begin{array}{lll}
\alpha_{\overline{\mathrm{MS}}}\left(m_{\mathrm{Z}}\right) & \text { 1-loop: } 0.11701 \\
& 2 & 0.00128 \\
& 3 & 0.00019 \\
& 4 & 0.00006
\end{array}
$$

uncertainty
estimate $=0.00025$

## Adding in c, b, t - quarks by perturbation theory (see later)

add charm
$\alpha_{\mathrm{s}}(\mu)$
0.4
$0.35-$
$0.3-$
$0.25-$
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$0.15-$
0.1
0.05
0
0
10

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uncertainty
estimate $=0.00025$

## Non-perturbative running of $\alpha_{S F}$





## Finite volume schemes

Boundary conditions matter in finite volume. Which ones?
A most relevant criterion is zero modes

- Zero modes of gauge fields
$\rightarrow$ perturbative expansion (+ MC)
- Zero modes of Dirac operator
$\rightarrow$ HMC stability


## Finite volume schemes

## Gauge field zero modes

Path integral w.o. fermions

$$
\begin{aligned}
\langle O(U)\rangle & =\frac{1}{\mathcal{Z}} \int \mathrm{D}[U] \mathrm{e}^{-\beta \bar{S}(U)} O(U) \\
\bar{S}(U) & =\sum_{p} \operatorname{tr}(1-U(p)), \quad \beta=\frac{6}{g_{0}^{2}}
\end{aligned}
$$

PT, sketchy

$$
\begin{aligned}
\beta \rightarrow \infty \quad & U \approx U_{\min } \equiv V \text { dominates (classical solution) } \\
& U(x, \mu)=V(x, \mu) \mathrm{e}^{\overline{\mathrm{b}}_{\mu}(x) T^{b}}, \quad \bar{q}_{\mu}^{b}(x) \ll 1, \quad \int \mathrm{D}[U] \rightarrow \int \mathrm{D}[\bar{q}] \\
\bar{S}(U)= & \bar{S}(V)+\sum_{n, m} q_{m} K_{m n} q_{n}+\mathrm{O}\left(q^{3}\right), \quad q_{n}=\bar{q}_{\mu}^{b}(x), n=\left(\frac{x}{a}, \mu, b\right) \\
O(U)= & O(V)+\ldots
\end{aligned}
$$

Gauss intergrals $\rightarrow$ Wick contractions ... IFF $K$ has no zero modes ( $K v=\lambda v, \lambda>0$ )

## Finite volume schemes

Generically there are zero modes
gauge modes $\rightarrow$ gauge fixing

- finite volume modes (gauge invariant)
"Ground state metamorhosis"[Gonzales Arroyo, Jurkiewicz, Korthals-Ates] with periodic BC's


## Finite volume schemes

## Ground state metamorphosis

Toy example: $\mathrm{SU}(2), L^{4}, L=a$ lattice, $\mathrm{PBC}, d=2$, single point

- $\bar{S}=2-\operatorname{tr}\left(U_{2} U_{1} U_{2}^{\dagger} U_{1}^{\dagger}\right)$
- $\operatorname{tr} U_{i}$ is gauge invariant, $U_{i}$ can't be gauged away
- minima: $U_{1}=U_{2}=V \ldots$ pick $U_{1}=U_{2}=1$.
- fluctuations $U_{i}=\mathrm{e}^{i \sigma^{b} q_{i}^{b}}$

$$
\bar{S}=2-\operatorname{tr}^{i \sigma^{b} q_{2}^{b}} \mathrm{e}^{i \sigma^{b} q_{1}^{b}} \mathrm{e}^{-i \sigma^{b} q_{2}^{b}} \mathrm{e}^{-i \sigma^{b} q_{1}^{b}}=\mathrm{O}\left(q^{4}\right) \quad \rightarrow K=0
$$

- $q=\mathrm{O}\left(\beta^{-1 / 4}\right)=\mathrm{O}\left(g_{0}^{1 / 2}\right)$

PT in powers of $g_{0}$, not $g_{0}^{2}$ NOT regular

- In general: mixture of gaussian and non-gaussian modes integrate over non-gaussian ones exactly ... complicated, non-universal $\beta$-function it can be worse, divergent behavior, $1 / \log (g)$ terms , see [Nogradi etal. 2012]
- think of these $U_{i}$ as Polyakov loops $\rightarrow$ relevant for 4-d gauge theory. "Ground state metamorhosis" $[$ Gonzales Arrove, Jurkiewicz, Korthals-Altes]


## Finite volume schemes

$$
V(x, \mu)=1, \quad \text { PBC: } \psi(x+L \hat{\mu})=\psi(x)
$$

massless Dirac operator has a zero mode (constant mode, $p=0$ ) easily fixed by

$$
\psi(x+L \hat{\mu})=\mathrm{e}^{i \alpha} \psi(x)
$$

e.g. $\alpha=\pi / 2$ in $\operatorname{SU}(2), \alpha=\pi / 3$ in $\operatorname{SU}(3)$

Exercise: why these values of $\alpha$ ?

## Finite volume schemes

## Schrödinger functional

## Boundary conditions

- Space: PBC
- Time: Dirichlet, breaks translation invariance!

Yang Mills theory [Luscher, Narayanan, Weisz \& Wolff]:


$$
\begin{aligned}
\mathcal{Z}\left(V, V^{\prime}\right) & =\int \mathrm{D}(U)_{\text {inside }} \mathrm{e}^{-S_{\mathrm{SF}}(U)} \\
S_{\mathrm{SF}}(U) & =\sum_{p \text { inside }} \beta \operatorname{tr}(1-U(p)), \quad U(x, k)= \begin{cases}V(\mathbf{x}, k) & x_{0}=0 \\
V^{\prime}(\mathbf{x}, k) & x_{0}=T\end{cases}
\end{aligned}
$$

Standard introduction of Hilbert space, transfer matrix:

$$
\mathcal{Z}\left(V, V^{\prime}\right)=\left\langle V^{\prime}\right| \underbrace{e^{-\hat{H} T}}_{\mathbb{T}^{T} / a} \underbrace{\mathbb{P}_{0}}_{\substack{\uparrow \\ \text { projector onto gauge invariant states }}}|V\rangle, \quad \hat{U}(\mathbf{x}, k)|U\rangle=U(\mathbf{x}, k)|U\rangle
$$

$\mathcal{Z}\left(V, V^{\prime}\right)=$ Euclidean time propagation kernel by time $T=$ Schrödinger functional

## Finite volume schemes

## Schrödinger functional : quarks

## Wilson Dirac operator (also others are possible)

$$
\begin{aligned}
& D_{\mathrm{W}}=\frac{1}{2}\left\{\gamma_{\mu}\left(\nabla_{\mu}+\nabla_{\mu}^{*}\right)-a \nabla_{\mu}^{*} \nabla_{\mu}\right\} \\
& \nabla_{\mu} \psi(x)=\frac{1}{a}[U(x, \mu) \psi(x+a \hat{\mu})-\psi(x)] \\
& \nabla_{\mu}^{*} \psi(x)=\frac{1}{a}\left[\psi(x)-U(x-a \hat{\mu}, \mu)^{-1} \psi(x-a \hat{\mu})\right]
\end{aligned}
$$

Schrödinger functional action

$$
\begin{aligned}
S_{\mathrm{F}}= & a^{4} \sum_{x} \bar{\psi}(x)\left[m_{0}+D_{\mathrm{W}}\right] \psi(x), \\
\text { with } & \psi(x)=0, \bar{\psi}(x)=0 \text { for } x_{0} \leq 0, \text { and } x_{0} \geq T
\end{aligned}
$$

In the continuum theory this corresponds to BC's [sint, 1994]

$$
\begin{array}{lll}
\left.P_{+} \psi(x)\right|_{x_{0}=0}=0 & \left.\bar{\psi}(x) P_{-}\right|_{x_{0}=0}=0 & P_{ \pm}=\frac{1}{2}\left(1 \pm \gamma_{0}\right) \\
\left.P_{-} \psi(x)\right|_{x_{0}=T}=0 & \left.\bar{\psi}(x) P_{+}\right|_{x_{0}=T}=0
\end{array}
$$

These BC's are stable: emerge in the cont. limit without fine-tuning. Universality! [Luscher, 2006] The Universality class is characterised by Parity invariance, discrete rot. invariance (not chiral symm).

## Finite volume schemes

Correlation functions can be formed with the usual fields in the interior (bulk) and the boundary quark fields

$$
\begin{array}{cl}
\zeta(\mathbf{x})=\left.P_{-} U(x, 0) \psi(x+a \hat{0})\right|_{x_{0}=0} & \bar{\zeta}(\mathbf{x})=\left.\bar{\psi}(x+a \hat{0}) P_{+} U(x, 0)^{-1}\right|_{x_{0}=0} \\
\zeta^{\prime}(\mathbf{x})=\left.P_{+} U(x-a \hat{0}, 0)^{-1} \psi(x-a \hat{0})\right|_{x_{0}=T} & \bar{\zeta}^{\prime}(\mathbf{x})=\left.\bar{\psi}(x-a \hat{0}) P_{-} U(x-a \hat{0}, 0)\right|_{x_{0}=T}
\end{array}
$$

A very interesting feature of these is that one can form correlation functions where the quark fields are projected to $\mathbf{p}=0$. (Note that the gauge fields at the boundaries are fixed).

$$
\begin{aligned}
f_{\mathrm{P}}^{r s}\left(x_{0}\right) & =a^{6} \sum_{\mathbf{v}, \mathbf{y}}\left\langle\bar{\zeta}_{s}(\mathbf{v}) \gamma_{5} \zeta_{r}(\mathbf{y}) P^{r s}(x)\right\rangle \\
P^{r s}(x) & =\bar{\psi}_{r}(x) \gamma_{5} \psi_{s}(x)
\end{aligned}
$$

## Finite volume schemes

## boundary quark fields

$$
\begin{array}{cl}
\zeta(\mathbf{x})=\left.P_{-} U(x, 0) \psi(x+a \hat{0})\right|_{x_{0}=0} & \bar{\zeta}(\mathbf{x})=\left.\bar{\psi}(x+a \hat{0}) P_{+} U(x, 0)^{-1}\right|_{x_{0}=0} \\
\zeta^{\prime}(\mathbf{x})=\left.P_{+} U(x-a \hat{0}, 0)^{-1} \psi(x-a \hat{0})\right|_{x_{0}=T} & \bar{\zeta}^{\prime}(\mathbf{x})=\left.\bar{\psi}(x-a \hat{0}) P_{-} U(x-a \hat{0}, 0)\right|_{x_{0}=T}
\end{array}
$$

These boundary quark fields renormalize multiplicatively.

$$
\zeta_{\mathrm{R}}(\mathbf{x})=Z_{\zeta} \zeta(\mathbf{x}), \ldots, \bar{\zeta}_{\mathrm{R}}^{\prime}=Z_{\zeta} \bar{\zeta}^{\prime}(\mathbf{x})
$$

Define also boundary-to-boundary correlation functions

$$
f_{1}^{r s}=\frac{a^{12}}{L^{6}} \sum_{\mathbf{v}, \mathbf{y}, \mathbf{u}, \mathbf{x}}\left\langle\bar{\zeta}_{s}(\mathbf{v}) \gamma_{5} \zeta_{r}(\mathbf{y}) \bar{\zeta}_{r}^{\prime}(\mathbf{u}) \gamma_{5} \zeta_{s}^{\prime}(\mathbf{x})\right\rangle
$$



Then

$$
\left(f_{1}^{r s}\right)_{\mathrm{R}}=Z_{\zeta}^{4}\left(f_{1}^{r s}\right), \quad\left(f_{\mathrm{P}}^{r s}\left(x_{0}\right)\right)_{\mathrm{R}}=Z_{\zeta}^{2} Z_{\mathrm{P}}\left(f_{\mathrm{P}}^{r s}\left(x_{0}\right)\right)
$$

## Finite volume schemes

- Regular PT (no gauge field zero modes)
- Gap for Dirac operators
- Momentum zero boundary quark fields (spatially one takes pbc up to a phase, cf "flavor twisted bc")
- Schrödinger functional coupling defined with non-trivial $V, V^{\prime}$ $\beta$-function known to 3-loops [Lnww: Lw; Bode, Weisz, Wolfi]


## Finite volume schemes

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- We can define $Z$-factors (schemes) for composite fields, e.g.

$$
Z_{\mathrm{P}}=\frac{1}{c(a / L)} \frac{\sqrt{f_{1}^{r s}}}{f_{\mathrm{P}}^{r s}(T / 2)}, \quad c(a / L)=\left.\frac{\sqrt{f_{1}^{r s}}}{f_{\mathrm{P}}^{r(T / 2)}}\right|_{g_{0}=0}
$$

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$$

- There is also a new SF coupling ...


## Exercise

Consider the free Schrödinger functional , i.e. $U(x, \mu)=1$ with pbc in space for the fermions.

- Show that $f_{\mathrm{P}}\left(x_{0}\right)=$ constant for mass-less quarks. hints:
- write down the Wick-contraction in terms of the Schrödinger functional propagator
- note that it is apropriate to go to momentum space concerning the space components, but to remain in coordinate space concerning the time coordinates
- what is the the equation for the spatial $\mathbf{p}=0$ contribution to the propagator? note how it splits into $P_{ \pm}$pieces
- solve the equation by "inspection", iteration
- obtain the result for arbitrary quark mass
- Could this result be guessed by dimensional reasoning?


## Gradient Flow and SF-coupling

- Gradient flow [Luscher, 2010; Luscher \& Weisz, 2011]
new observables
- UV finite (proven to all orders of PT)
- excellent numerical precision
- renormalized coupling in finite volume with pbc [вмш, 2012]
- Flow in finite volume, SF [p. Fritzsch \& Ramos, arxiv: 1301.4388]
- lowest order PT to define a new coupling
- numerical investigation shows excellent precision
- Flow with gauge fields AND quark fields [Lüscher,arxiv: 1302.5246]
- General idea

$$
\begin{aligned}
& x=\left(x_{0}, \mathbf{x}\right), \quad t=\text { flow time } \\
& A_{\mu}(x)=\text { quantum gauge fields : } \mathcal{Z}=\int \mathrm{D}\left[A_{\mu}(x)\right] \ldots \\
& B_{\mu}(x, t)=\text { smoothed gauge fields }, \quad B_{\mu}(x, 0)=A_{\mu}(x) \\
& \frac{\mathrm{d} B_{\mu}(x, t)}{\mathrm{d} t}=D_{\nu} G_{\nu \mu}(x, t)+\text { gauge fixing } \\
& \sim-\frac{\delta S_{Y M}[B]}{\delta B_{\mu}}
\end{aligned}
$$

correlation functions of $B$-fields at arbitrary points are finite

## Gradient Flow

- in PT: $A_{\mu}(x)=g_{0} \bar{A}_{\mu}(x)$

$$
\begin{aligned}
B_{\mu}(x, t)= & B_{\mu, 1}(x, t) g_{0}+B_{\mu, 2}(x, t) g_{0}^{2}+\ldots \\
& G_{\nu \mu}=\left[\partial_{\nu} B_{\mu, 1}-\partial_{\mu} B_{\nu, 1}\right] g_{0}+\mathrm{O}\left(g_{0}^{2}\right), \quad D_{\nu}=\partial_{\nu}+\mathrm{O}\left(g_{0}\right) \\
\rightarrow \quad \dot{B}_{\mu, 1}(x, t)= & \partial_{\nu} \partial_{\nu} B_{\mu, 1}(x, t)
\end{aligned}
$$

- heat equation

$$
\begin{aligned}
B_{\mu, 1}(x, t)= & \int \mathrm{d}^{D} p \mathrm{e}^{i p x} b_{\mu}(p, t) \\
& \dot{b}_{\mu}=-p^{2} b_{\mu} \rightarrow b_{\mu}(p, t)=b_{\mu}(p, 0) \mathrm{e}^{-p^{2} t} \\
B_{\mu, 1}(x, t)= & \int \mathrm{d}^{D} y K_{t}(x-y) \bar{A}_{\mu}(y), \quad K_{t}(z)=(4 \pi t)^{-D / 2} \mathrm{e}^{-z^{2} /(4 t)}
\end{aligned}
$$

- smoothing over a radius of $\sqrt{8 t}$
- gaussian damping of large momenta


## Gradient Flow

$\Rightarrow$ in PT: $A_{\mu}(x)=g_{0} \bar{A}_{\mu}(x)$

$$
\begin{aligned}
B_{\mu}(x, t)= & B_{\mu, 1}(x, t) g_{0}+B_{\mu, 2}(x, t) g_{0}^{2}+\ldots \\
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B_{\mu, 1}(x, t)= & \int \mathrm{d}^{D} y K_{t}(x-y) \bar{A}_{\mu}(y), \quad K_{t}(z)=(4 \pi t)^{-D / 2} \mathrm{e}^{-z^{2} /(4 t)}
\end{aligned}
$$

- smoothing over a radius of $\sqrt{8 t}$
- gaussian damping of large momenta
- all correlation functions of $B_{\mu}$ are finite $(t>0)$ [Luscher \& Weisz, 2011] in particular $\langle E(t)\rangle, \quad E(t)=-\frac{1}{2} \operatorname{tr} G_{\mu \nu} G_{\mu \nu}$


## Gradient Flow

## Yang-Mills theory

- order by order iteration:

$$
\begin{aligned}
& B_{\mu}(x, t)=\sum_{k} B_{\mu, n}(x, t) g_{0}^{k} \\
& \dot{B}_{\mu, k}(x, t)-\partial_{\nu} \partial_{\nu} B_{\mu, k}(x, t)=R_{\mu, k} \\
& R_{\mu, 1}=0, \quad B_{\mu, 1}(x, t)=\int \mathrm{d}^{D} y K_{t}(x-y) \bar{A}_{\mu}(y) \\
& R_{\mu, 2}=2\left[B_{\nu, 1}, \partial_{\nu} B_{\mu, 1}\right]-\left[B_{\nu, 1}, \partial_{\mu} B_{\nu, 1}\right] \\
& R_{\mu, 3}=2\left[B_{\nu, 2}, \partial_{\nu} B_{\mu, 1}\right]+2\left[B_{\nu, 1}, \partial_{\nu} B_{\mu, 2}\right] \\
& \quad \quad-\left[B_{\nu, 2}, \partial_{\mu} B_{\nu, 1}\right]-\left[B_{\nu, 1}, \partial_{\mu} B_{\nu, 2}\right]+\left[B_{\nu, 1},\left[B_{\nu, 1}, B_{\mu, 1}\right]\right], \\
& \ldots \\
& B_{\mu, k}(t, x)=\int_{0}^{t} \mathrm{~d} s \int \mathrm{~d}^{D} y K_{t-s}(x-y) R_{\mu, k}(s, y) \quad k>1
\end{aligned}
$$

## Gradient Flow

## Yang－Mills theory

－order by order iteration：

$$
\begin{aligned}
& B_{\mu}(x, t)=\sum_{k} B_{\mu, n}(x, t) g_{0}^{k} \\
& \dot{B}_{\mu, k}(x, t)-\partial_{\nu} \partial_{\nu} B_{\mu, k}(x, t)=R_{\mu, k} \\
& R_{\mu, 1}=0, \quad B_{\mu, 1}(x, t)=\int \mathrm{d}^{D} y K_{t}(x-y) \bar{A}_{\mu}(y) \\
& R_{\mu, 2}=2\left[B_{\nu, 1}, \partial_{\nu} B_{\mu, 1}\right]-\left[B_{\nu, 1}, \partial_{\mu} B_{\nu, 1}\right], \\
& R_{\mu, 3}=2\left[B_{\nu, 2}, \partial_{\nu} B_{\mu, 1}\right]+2\left[B_{\nu, 1}, \partial_{\nu} B_{\mu, 2}\right] \\
& \quad \quad-\left[B_{\nu, 2}, \partial_{\mu} B_{\nu, 1}\right]-\left[B_{\nu, 1}, \partial_{\mu} B_{\nu, 2}\right]+\left[B_{\nu, 1},\left[B_{\nu, 1}, B_{\mu, 1}\right]\right], \\
& \ldots \\
& B_{\mu, k}(t, x)=\int_{0}^{t} \mathrm{~d} s \int \mathrm{~d}^{D} y K_{t-s}(x-y) R_{\mu, k}(s, y) \quad k>1
\end{aligned}
$$

－For $\langle E\rangle, E=-\frac{1}{2} \operatorname{tr} G_{\mu \nu} G_{\mu \nu}$

$$
\begin{aligned}
\langle E\rangle= & E_{0} g_{0}^{2}+E_{0} g_{0}^{4}+\ldots \\
E_{0}= & \left\langle\operatorname{tr}\left[\partial_{\mu} B_{\nu, 1} \partial_{\mu} B_{\nu, 1}-\partial_{\mu} B_{\nu, 1} \partial_{\nu} B_{\mu, 1}\right]\right\rangle \\
& \sim \int_{p} \mathrm{e}^{-p^{2} 2 t}\left[p^{2} \delta_{\mu \nu}-p_{\mu} p_{\nu}\right] D_{\mu \nu}(p) \text { finite (also with cutoff reg'n)! }
\end{aligned}
$$

## Gradient Flow and SF-coupling

use the flow in SF: $T \times L^{3}$ world with Dirichlet BC in time, $T=L$ define

$$
\begin{aligned}
\langle E(t)\rangle & \equiv-\frac{1}{2}\left\langle\operatorname{tr} G_{\mu \nu} G_{\mu \nu}(x, t)\right\rangle_{x_{0}=T / 2}=\frac{\mathcal{N}}{t^{2}} \bar{g}_{\mathrm{MS}}^{2}(\mu)\left(1+c_{1} \bar{g}_{\mathrm{MS}}^{2}+\ldots\right) \\
\bar{g}_{\mathrm{GF}}^{2}(L) & \left.\equiv \mathcal{N}^{-1} t^{2}\langle E(t)\rangle\right|_{t=c^{2} L^{2} / 8}
\end{aligned}
$$

This is a family of schemes characterized by $c$ (dimensionless)

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\bar{g}_{\mathrm{GF}}^{2}(L) & \left.\equiv \mathcal{N}^{-1} t^{2}\langle E(t)\rangle\right|_{t=c^{2} L^{2} / 8}
\end{aligned}
$$

This is a family of schemes characterized by $c$ (dimensionless)

$$
\begin{aligned}
\mathcal{N}(c)= & \frac{c^{4}\left(N^{2}-1\right)}{128} \sum_{\mathbf{n}, n_{0}} e^{-c^{2} \pi^{2}\left(\mathbf{n}^{2}+\frac{1}{4} n_{0}^{2}\right)} \\
& \times \frac{2 \mathbf{n}^{2} s_{n_{0}}^{2}(T / 2)+\left(\mathbf{n}^{2}+\frac{3}{4} n_{0}^{2}\right) c_{n_{0}}^{2}(T / 2)}{\mathbf{n}^{2}+\frac{1}{4} n_{0}^{2}}
\end{aligned}
$$

- the lattice version is known (and needed)


## Gradient Flow and SF-coupling

## statistical precision: variance

$$
\text { relative variance }=\frac{\left\langle E^{2}\right\rangle-\langle E\rangle^{2}}{\langle E\rangle^{2}}
$$

should be finite as $a \rightarrow 0, L / a \rightarrow \infty$
Numerically, Fritzsch \& Ramos:


## Gradient Flow and SF-coupling

## statistical precision

autocorrelations scale as expected: $\tau_{\text {int }} \propto a^{-2}$


Statistical precision is good and theoretically understood. There will be no surprises on the way to the continuum limit.

