Scale Setting in Lattice QCD

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Lattice 2013, Mainz, July 2013



- M. Lüscher
 - ... for very useful corresponence & SU(3) YM data
- Gregorio Herdoiza ...for graphs and discussion
- BMW, Nathan Brown, Albert Deuzeman, Georg von Hippel, Roger Horsley, Björn Leder, Harvey Meyer, Albert Ramos, Carsten Urbach ... for material, data, graphs

For illustration I use mainly plots from ALPHA: M. Bruno & S. Lottini !

What is scale setting



Simplification: ignore QED and Isospin splitting

- N_f parameters, g_0^2 , $m_u = m_d$, m_s ...
- ► Need to fix Φ_i , $i = 1 ... N_f$ dimensionless quantities to take a continuum limit and in the end to have real world QCD (e.g. up to $O(\Lambda/m_c)$)
- hadronic input

$$m_1^{\rm h} = m_\pi \,, \; m_2^{\rm h} = m_{\rm K} \,, \; (m_3^{\rm h} = m_{\rm D} \,, \; m_4^{\rm h} = m_{\rm B})$$

- + a scale
- Length scale

 $\label{eq:Q} \begin{array}{l} Q \ , \ [Q] = -1 \\ \Phi_i = Q \, m_i^{\rm h} \mbox{ dimensionless} \end{array}$

Natural from the physics point of view:

$$Q = m_{\rm proton}^{-1}$$

or

$$Q = f^{-1}$$

(low energy constant of SU(2) chiral Lagrangian)

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- check for cutoff effects
- decouple scale setting from the rest of the calculation e.g. compute $B \rightarrow \pi$ form factor ...
- fix quark masses from the beginning
- There have been changes in predictions due to better determinations of the scale



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HPQCD, 2007 $f_{D_s} = 241(3) \text{ MeV}$ scale from $r_1 = 0.321(5)$ HPQCD, 2010 $f_{D_s} = 248.0(2.5) \text{ MeV}$ scale from $r_1 = 0.3133(23)$

• Example 2:
$$\Lambda_{\overline{\mathrm{MS}}}$$
, $N_{\mathrm{f}}=2$

 $\begin{array}{lll} \mbox{ALPHA, 2004} & \Lambda_{\overline{\rm MS}} = 245(16)(16)\,{\rm MeV} & \mbox{scale from QCDSF}\ (r_0 \approx 0.5\,{\rm fm}) \\ \mbox{ALPHA, 2012} & \Lambda_{\overline{\rm MS}} = 310(20)\,{\rm MeV} & \mbox{scale from ALPHA}\ (\ f_{\rm K}\) \end{array}$



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It is important to have a precise and correct scale determination.

Criteria



Criteria for a good \boldsymbol{Q}

- Precision
 - statistical

related!

- systematic
- Quark mass dependence
 - weak dependence is better: it is easier to fix the scale at $(m_{\rm PS},m_{\rm K})=(m_\pi^{\rm phys},m_{\rm K}^{\rm phys})$
- N_f dependence
 - first we need to define this...



Hadronic, experimentally measurable

$\blacktriangleright m_{\Omega}$

- stable, best S/N ratio of non pseudo scalars
- f_{π}, f_{K}
 - pseudo scalar: very good S/N
 - but knowledge of V_{ud} , (or V_{us}) assumed

Constructed (only we can say what their values are precisely)

- \succ r_0, r_1 (static force)
 - still linked to phenomenology (a bit dirty)
 - solvable S/N problem (in practise)
- t_0, w_0 (gradient flow)
 - artificial
 - very precise

Once r_0, r_1, w_0, w_1 are determined from hadronic quantities, they are just as good (or better).

Being established

- v_0 (my name)
 - from Isospin 1 hadronic vacuum polarisation
 - Harvey Meyer

Vector correlator and scale determination in lattice QCD Mon, 14:40, Seminar Room C (RW4)

Harvey Meyer

Vector correlator and scale determination in lattice QCD Mon, 14:40, Seminar Room C (RW4)

Mattia Bruno

On the Nf-dependence of gluonic observables Mon, 15:00, Seminar Room C – Parallels 1C

Nathan Brown

Symanzik flow on HISQ ensembles Mon, 18:10, Seminar Room G (HS III)

Roger Horsley

SU(3) flavour symmetry breaking and charmed states Thu, 15:20, Seminar Room G – Parallels 7G





Reasonable signal-to-noise ratio

 $\begin{array}{l} \mathsf{BMW:}\ 2+1 \ \text{``HEX''}\\ a\approx 0.054 \ \text{fm}, m_{\pi}\approx 260 \text{MeV}, L\approx 1.7 \text{fm} \end{array}$



aparently very uncorrelated data

Mainz group, CLS configurations, $N_{\rm f} = 2$ $a \approx 0.045 \text{ fm}, m_{\pi} \approx 340 \text{MeV}, L \approx 2.2 \text{fm}$





f_{π}, f_{K}

- good signal-to-noise
- small \(\tau_{int}\) quite weak coupling to slow modes

autocorrelation function of f_{π}

 $a=0.045~{
m fm},$ large statistics ~
ightarrow

tail contributes \approx 20 MDU to $\tau_{\rm int}$

significant dependence on either light quark masses: f_{π} or strange quark mass: $f_{\rm K}$

We do have ChPT for the asymptotic behavior

light quark mass dependence for $N_{\rm f}=2$:



Figures: S. Lottini, ALPHA

r_0 , r_1 , the all-time favorites





Issues

- V(r) from large T behavior of Wilson loop (variationally improved)
 F(r_I) by an interpolation
 - instead: force often through fits to V(r) over a larger range of r
 - ightarrow what excatly one determines depends on the assumed shape (fitfunction)
- Signal-to-noise problem

- $\frac{\text{signal}}{\text{noise}}(\text{Wloop}) \sim \exp(-\frac{e_1}{a} + \text{finite}T)$
- grows towards the continuum limit
- *e*¹ can be reduced by a change of static quark action

A. Hasenfratz & F. Knechtli, 2003; M. Della Morte, A. Shindler & R.S. 2005

• r_1 was motivated by an improvement of the signal but: shorter distance, larger discretisation effects amazing: MILC lattices: r_1/a down to $r_1/a = 2$

MILC, 2000

A modern computation of r_0



M. Donnellan, F. Knechtli, B. Leder and R. S., ALPHA (2010) On CLS ensembles, $N_{\rm f} = 2$ Basis of (smeared) parallel transporters, GEVP M. Lüscher & U. Wolff, 1991 fixed $r \approx r_0$: $C(t) \psi_{\alpha} = \lambda_{\alpha}(t, t_0) C(t_0) \psi_{\alpha}, \quad \alpha = 0 \dots M - 1$ 0.398 fit of effective mass plateau average GEVP, r/a = 7, $t_0/a = 2$ 0.396 $E_{\alpha}(t,t_0)$ GEVP, r/a = 7, $t_0/a = 5$ $\equiv \ln \left(\lambda_{\alpha}(t, t_0) / \lambda_{\alpha}(t + a, t_0) \right)$ 0.394 $= E_{\alpha} + \beta_{\alpha} \mathrm{e}^{-(E_M - E_{\alpha})t}$ $E_0(t, t_0)$ 265'0 0.39 Not entirely trivial But here solved 0.388 Important: understanding of the corrections! 0.386 2 12 4 6 8 10 14 16 Collaboration, Blossier et al., 2009 t/a

Quark mass dependence of r_0





- Weak dependence on quark mass.
- > ETMC quark mass dependence seems even weaker at larger lattice spacings.



$N_{\rm f}$	r_0 [fm]	Reference	
2 2 2 2 2 2 2 2 2	$\begin{array}{c} 0.420(20)\\ 0.465(15)\\ 0.438(14)\\ 0.450(15)\\ 0.503(10)\\ 0.485(9)\\ 0.491(6)\end{array}$	ETMC 08 from f_{π} ETMC 09 from $m_{nucleol}$ ETMC 09 from f_{K} ETMC from f_{π} Lat13 ALPHA from f_{π} Lat13 ALPHA from f_{π} Lat13 ALPHA from f_{K} Lat13	
3	0.480(11)	RBC 12	⊢ ••••
		-	0.4 0.42 0.44 0.46 0.48 0.5

æ

$t_0, w_0,$ the newcomers Gradient flow

Gradient flow

- New renormalised observables depending on $t \neq x_0, t > 0$
 - Flow equation $B_{\mu}(x,t)$ with $B_{\mu}(x,0) = A_{\mu}$ = quantum field

$$\frac{\mathrm{d}}{\mathrm{dt}}B_{\mu}(x,t) = \dot{B}_{\mu}(x,t) = D_{\nu}G_{\nu\mu}(x,t) \sim -\frac{\delta S_{YM}[B]}{\delta B_{\mu}}$$

• smoothing over a radius of $\sqrt{8t}$, lowest order of PT:

$$B_{\mu}(x,t) = \int d^{4}y \ (4\pi t)^{-2} e^{-(x-y)^{2}/(4t)} \ A_{\mu}(y) + O(g_{0}^{2})$$

- Discretisation of the flow equation
 - "Wilson flow"

$$\dot{V}(t) = -\frac{\partial}{\partial V} S_{\rm plaq}(V) V(t) \,, \qquad V(0) = U$$

"Symanzik flow"

$$\dot{V}(t) = -\frac{\partial}{\partial V} S_{\text{TLSymanzik}}(V) V(t), \qquad V(0) = U$$

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M. Lüscher, 2010



5-d formulation

M. Lüscher and P. Weisz, 2010, M. Lüscher 2012

- $t \ge 0$ as additional coordinate [t]=length²
- 4-d field theory at t = 0 boundary
- For precise understanding of renormalisation and improvement

$$E(x,t) = -\frac{1}{4} \operatorname{tr} G_{\mu\nu}(x,t) G_{\mu\nu}(x,t)$$

Observation in numerical data:

$$t^2 \langle E(t) \rangle \approx k t$$
 for $t = O(r_0^2)$
 $t_0^2 \langle E(t_0) \rangle = 0.3$ defines t_0

Discretisations in use

- E = plaquette
- $G_{\mu\nu}$ = clover (" symmetric ")



E





M. Lüscher, 1006.4518

Definition

BMW, 1203.4469

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Scale through m_{Ω}



1203.4469: $t^2 \langle E(t) \rangle$: "scales between a and \sqrt{t} " w_0 : "scales of order w_0 only"

however: leading order of PT:

$$\begin{split} \langle E(t) \rangle &\sim g^2 \int \mathrm{d}^4 p \mathrm{e}^{-2tp^2} (p^2 \delta_{\mu\nu} - p_\mu p_\nu) D(p)_\mu \\ t^2 \langle E(t) \rangle &\sim g^2 \int_0^\infty p^3 \mathrm{e}^{-2tp^2} \mathrm{d}p \\ t \partial_t [t^2 \langle E(t) \rangle] &\sim g^2 \int_0^\infty p^3 \left(1 - t \, p^2\right) \mathrm{e}^{-2tp^2} \mathrm{d}p \end{split}$$



Integrands in LO PT vs. $p\sqrt{t}$



The possible interest is in a^2 improvement

For that one needs

- improvement of 4-d action
- improvement of the flow equation (no g₀² dependence) (t > 0 bulk of 5d theory)
- improvement of flow observables, E (no g₀² dependence) (t > 0 bulk of 5d theory)

boundary improvement terms such as

$$a^6 \sum_x \partial_t \operatorname{tr} G_{\mu\nu} G_{\mu\nu}|_{t=0}$$

at the t = 0 boundary

Incomplete improvement may be worse than no improvement

Flow quantities (and in general)

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Incomplete improvement can be worse than no improvement

- a² improvement of 4-d action, i.e. tree-level Symanzik action
- but no improvement

of flow observables, E



Here: Plaquette action is better than tree level improved (LW).

t_0, w_0 statistical precision

Very small and scaling variance.

Strong coupling to slow modes of HMC. (\rightarrow perfect detector of slow modes)



$$N_{
m f}=2~$$
 [M. Bruno, ALPHA, 2013]

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$$a = 0.075 \,\mathrm{fm}$$

 $m_{\pi} = 280 \,\mathrm{MeV}$

 $a = 0.049 \,\mathrm{fm}$ $m_{\pi} = 340 \,\mathrm{MeV}$

- All in all excellent precision.
- No relevant differences between t_0 and w_0 .

- ALPHA (2): $\tau_{int} \approx 50...130 \text{ MDU}$ a = 0.049...0.075 fm
- ▶ BMW (2+1, 2HEX): $\tau_{int} \approx 70 \text{ MDU}$ $a \ge 0.054 \text{ fm}$
- MILC (2+1+1, HISQ): $\tau_{int} \approx 20...80$ MDU a = 0.06...0.15 fm

t_0, w_0 : quark mass dependence







- very linear
- but we have no theory for asymptotic behavior (ChPT)
- comment: no (mass-dependent) discretisation effects visible (e.g. due to missing b_g-terms) with precise data

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July, 30, 2013

t_0, w_0 : quark mass dependence

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 $N_{\rm f} = 2 + 1$, QCDSF, tr $m_{\rm quark}$ =const. $N_{\rm f} = 2$ [ALPHA, 2013] & $y = t_0(m) m_\pi^2 \sim m_{\text{quark}}$ $w_0^2(y)/w_0^2(0.8)$ $t_0(y)/t_0(0.8)$ 1.15 1.08 QCDSF, tr M=const. QCDSF, tr M=const 1.06 β=5.2 -1.1 $\beta = 5.2$ 1.04 1.02 v₀²(y)/w₀²(0.08) 1.05 β=5.5 ----₀(y)/t₀(0.08) 1 0.98 0.96 L 0.95 0.94 0.92 0.9 09 0.85 0.88 0.02 0.04 0.06 0.08 0.1 0.12 0.14 0.16 0.18 0 0.02 0.04 0.06 0.08 01 0 12 0 14 0 16 0 18 y tr m_{quark} =const.: rather flat behavior in agreement with $t_0(y) = t_0(y_{sym}) + O((y - y_{sym})^2)$ where "sym" means $m_1 = m_2 = m_3$ see: Roger Horsley

SU(3) flavour symmetry breaking and charmed states Thu, 15:20, Seminar Room G - Parallels 7G

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July, 30, 2013

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- What do we mean by an N_f-dependence?
- Different N_f: different theory, different coupling ...

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► Related by decoupling, up to a change of the coupling ↔ a change of the scale (effective theory) Need to consider dimensionless low energy quantities

$$\begin{split} &R_{x,y}, \text{ nere } R_{t_0,r_0^2} = t_0/r_0^* \text{ etc.} \\ & m_{N_{\rm f}} \gg m_{N_{\rm f}-1} > \dots \\ & R_{x,y}^{(N_{\rm f})}(m_1,\dots,m_{N_{\rm f}}) = R_{x,y}^{(N_{\rm f}-1)}(m_1,\dots,m_{N_{\rm f}}-1) + \mathcal{O}((m_{N_{\rm f}})^{-k}), \quad k \geq 1 \end{split}$$

 N_f-dependence and quark mass dependence are related

N_f dependence





- Significant differences in gluonic scales between $N_{\rm f} = 0$ and 2
- which reduce when you increase the quark mass in $N_{\rm f}>2$
- Small differences for $N_{\rm f} > 2$

 $N_{\rm f} = 0 \langle E(t) \rangle$ data by M. Lüscher

• $N_f = 2 + 1$		• $N_f = 2 + 1 + 1$			
	Quantity [fm]	ref.	Quantity	ref.	
	$ \begin{aligned} r_0 &= 0.480(10)(4) \\ \sqrt{t_0} &= 0.1465(21)(13) \\ w_0 &= 0.1755(18)(4) \end{aligned} $	RBC, '12 BMW, '12 BMW, '12	$r_0/r_1 = 1.508 \sqrt{t_0}/w_0 = 0.835(8) r_1/w_0 = 1.790(25)$	HotQCD, '11 HPQCD, '13 HPQCD, '13	
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$\sqrt{t_0}$, w_0 in physical units

Uncertainties dominated by

- the physical observables used to set the scale
- the extrapolations to the physical point

N_{f}	$\sqrt{t_0}$ [fm]	w_0 [fm]	Reference		
0 2 3	$\begin{array}{c} 0.1630(10) \\ 0.1539(12) \\ 0.1530 \end{array}$	$0.1670(10) \\ 0.1760(13) \\ 0.1790$	$r_0 = 0.49 \mathrm{fm}$ Lat13* ALPHA from f_{K} Lat13 QCDSF from Octet Lat13		
3	0.1465(25)	0.1755(18)	BMW 12		H#H
4	0.1420(8)	0.1715(9)	HPQCD 13	Iel	HH
4		0.1712(6)	MILC from f_{π} Lat13		м
				0.14 0.145 0.15 0.155 0. t. [fm]	16 0.165 0.17 0.175 0. w. [fm]

* $N_{\rm f} = 0$: E(t) data of M. Lüscher [1006.4518]

- some VERY small uncertainties are being cited f_π to 0.3% including FSE, effects of strange tuning, charm tuning
- Some numbers are preliminary; should be discussed at Lat14



Quark mass dependence (roughly extracted): consider $t_0(m_{\pi}), w_0(m_{\pi})$

N_{f}	$rac{t_0(500 { m MeV})}{t_0(0)} - 1$	$rac{w_0^2(500{ m MeV})}{w_0^2(0)}-1$	Reference
2	-12%	-20%	ALPHA @ Lat13
2+1		-18%	BMW 2012
2+1+1		-13%	MILC Lat13



Lattice spacing dependence (roughly extracted) $t_0(a)$, $w_0(a)$

clover discretisation of $G_{\mu\nu}$

$N_{ m f}$	$rac{t_0(0.1{ m fm})}{t_0(0)} - 1$	$rac{w_0^2(0.1{ m fm})}{w_0^2(0)}-1$	ref.scale	Reference
0 2 2+1 2+1+1 2+1+1	-1% -8% -19%	$\begin{array}{l} \textbf{-3\%}\\ \textbf{-19\%}\\ \approx 0\\ \approx 0\\ \approx 0\\ \approx 0 \end{array}$	$r_0 \ r_0 \ m_\Omega \ f_\pi \ f_\pi$	Lat13 [data: 1006.4518] ALPHA @ Lat13 BMW 2012 HPQCD 13 MILC Lat13

This depends on many parameters:

4 - d action, boundary terms, flow equation, discretisation of $G_{\mu\nu}$, ref.scale Not surprisingly: see various numbers.



A Problem: r_0 for $N_{\rm f} = 2$

There were differences: r_0 , $N_f = 2 \text{ ETMC}$



light color: $3.5 \lesssim m_{\pi}L < 4$

A Problem: r_0 for $N_{\rm f} = 2$



There were differences: r_0 , $N_f = 2 \text{ ETMC}$ vs. ALPHA



light color: $3.5 \lesssim m_{\pi}L < 4$

Results for $f_{\pi}(m) r_0(m)$, $N_{\rm f} = 2$



raw data for ETMC[0911.5061] and ALPHA [Lat13] plot against $y = (m_{\pi}^+/f_{\pi}^+)^2/(8\pi^2)$



At fixed mass



... but they cross

G. Herdoiza, S. Lottini, ALPHA + ETMC, Lat13

interpolated to fixed reference quark masses, e.g. by $m_{\pi}^2 r_0^2$ =fixed



Is this data ready for continuum extrapolations?

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interpolated to fixed reference quark masses, e.g. by $m_\pi^2 \, r_0^2$ =fixed



- Is this data ready for continuum extrapolations?
- There are better quantities; on the right r_0 does not enter and it is a 500MeV m_{π}
- ETMC: small differences when r_0 does not enter.
- But: maybe differences are there for small masses.



To twist or not to twist or how to twist



O(a) improved fermions	twisted mass fermions
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NP determination of c_{sw} tune to maximal twist NP determination of $c_A, Z_A \dots$ isospin breaking

Effects of isospin breaking



The splitting

$$\Delta m_{\pi}^2 = (m_{\pi}^0)^2 - (m_{\pi}^+)^2 \,,$$

was summarised in 1303.3516 [ETMC, G. Herdoiza, K. Jansen, C. Michael, K. Ottnad & C. Urbach].



Decay constant at NLO WChPT w. isospin breaking



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This motivates to use power counting $m_{\rm quark}\sim a^2\Lambda_{\rm QCD}^4$ [o. Bar, 2010] in WChPT:

$$f_{\pi}^{+} = f \left(1 - (y_{+} \log(y_{+}) + y_{0} \log(y_{0})) + \underbrace{\alpha}_{\text{LEC}} (y_{+} + y_{0}) + \mathcal{O}(y^{2}) \right)$$
$$y_{c} = \frac{(m_{\pi}^{c})^{2}}{16\pi^{2}f^{2}} = \frac{(m_{\pi}^{c})^{2}}{16\pi^{2}f_{\pi}^{+2}} + \mathcal{O}(m_{\text{quark}}^{4})$$

This suggests to use as a variable (e.g. in plots)

1

$$y_{\text{eff}}$$
: $y_{\text{eff}} \log(y_{\text{eff}}) \equiv \frac{y_+ \log(y_+) + y_0 \log(y_0)}{2}$

with a ChPT prediction

$$f_{\pi}^{+} = f \left(1 - 2y_{\text{eff}}\log(y_{\text{eff}}) + \alpha y_{\text{eff}} + \operatorname{tiny} + \mathcal{O}(y^{2})\right)$$

Decay constant



Plot $r_0 f_{\pi}^+$ against y_{eff} .



"error bars": half of difference $y - y_{eff}$

applied also NLO FS correction [G. Colangelo & U. Wenger, 2010; O. Bär, 2010] (not so important)

NLO WChPT with m_{quark} ∼ a²Λ⁴_{QCD} does not seem to capture the effect !
 Large other (additional) a² effects would be needed.

Decay constant



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- ▶ NLO WChPT with $m_{\text{quark}} \sim a^2 \Lambda_{\text{QCD}}^4$ does not seem to capture the effect !
- Large other (additional) a² effects would be needed.
- or the isospin splitting is not as large as usually thought the determination of m_{π}^0 is a difficult computation



The isospin-splitting seems not to be as big as often said (measurement of m⁰_π is very difficult)

Motivation

for $N_{\rm f}=2$ is fading away ... will there be work on the problem?

Replace

 r_0 by t_0, w_0 to gain statistical precision!!

Ultimately:

reduce the lattice spacing

Wishfull

thinking: a computation differing ONLY by the twist angle.



- Intermediate and relative scale setting
 - Wilson flow observables are very precise
 - Gluonic observables, no inversions, no valence quark mass dependences
 - We have t_0, w_0
 - there is little obvious difference
 - there are probably other useful quantities
 - cutoff effects are non-universal
 - a distinction between t_0 and w_0 is not clear
 - The $N_{\rm f}$ dependence of w_0 is weaker than the one of t_0
 - The use of r_0 , r_1 will slowly fade away in favor of t_0 , w_0 (and maybe others)



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- Hadronic scales
 - f_π seems the best but is dependent on V_{ud}
 - *m*_Ω appears fine
 - the isovector vector correlator is being developed
 - m_{P} would be nice \leftarrow solve signal/noise problem



 $r_0 f_{\pi}^+$ against y_{eff}

Assume reduced splitting by a factor 4: $A, B \rightarrow A/4, B/4$



"error bars": half of difference $y - y_{eff}$

applied also NLO FS correction [G. Colangelo & U. Wenger, 2010; O. Bär, 2010]

(not so important)

This looks more reasonable.