Comparison of lattice definitions of the topological charge

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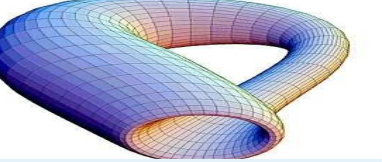
Presentation outline

1. Introduction
   - Motivation
   - Short overview of employed definitions
2. Results
   - Comparison at a single lattice spacing
   - Increase of correlation towards the continuum limit
   - Topological susceptibility
3. Conclusions



Motivation

Presentation outline

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Spectral projectors
Fermionic disc.
Field theoretic
Lattice setup

Results

Conclusions

- theoretical
  - ⋆ there are many definitions of the topological charge
  - ⋆ which of them should one use for different purposes?
    - ◇ to compute the topological susceptibility
    - ◇ to sort configurations according to the topological charge
    - ◇ for weighting results with the topological charge
  - ⋆ what are the pros and cons of different definitions?
  - ⋆ which definitions are theoretically clean and which are "suspicious"?
- practical
  - ⋆ quite a lot of data for the topological charge from different definitions and several projects

Definitions

- index of the overlap Dirac operator [K.C., E. García Ramos, K. Jansen]
- spectral flow of the Hermitian Wilson-Dirac operator [U. Wenger]
- spectral projectors [K.C., E. García Ramos, K. Jansen]
- fermionic from disconnected loops [C. Michael, K. Ottnad, C. Urbach, F. Zimmermann]
- field theoretic with HYP smearing [U. Wenger, F. Zimmermann]
- field theoretic with APE smearing [A. Dromard, M. Wagner, F. Zimmermann]
- field theoretic with cooling [A. Dromard, M. Wagner]
- field theoretic with gradient flow [U. Wenger]

Index of the overlap Dirac operator

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- Chirally symmetric fermionic discretizations allow exact zero modes of the Dirac operator.
- The famous Atiyah-Singer index theorem [M. Atiyah, I.M. Singer, Ann. Math. 93, 139 (1971) 168] relates the topological charge to the number of zero modes of the Dirac operator:

$$Q = n_- - n_+$$

- This is quite remarkable, because a property of gauge fields is linked to a fermionic observable.
- uniqueness: dependence on the s parameter of the kernel
  warning: locality [K. C., V. Drach, E. García Ramos, G. Herdoiza, K. Jansen, Nucl.Phys. **B**869 (2013) 131-163, arXiv:1211.1605 [hep-lat]]
- pros: theoretically clean, integer-valued, no renormalization
- cons: cost, cost, cost...

Spectral flow of the Hermitian Wilson-Dirac operator

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- closely related and actually equivalent to the index
- uniqueness: dependence on the s parameter of the kernel
- pros: theoretically clean, integer-valued, no renormalization, one computation leads to the whole s-dependence of the index
- cons: cost (although still cheaper than index), non-trivial to analyze data

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Spectral projectors

- another fermionic definition, introduced in:
  [L. Giusti, M. Lüscher, 2008], [M. Lüscher, F. Palombi, 2010]
- $\mathbb{P}_M$ – projector to the subspace of eigenmodes of $D^\dagger D$ with eigenvalues below M^2, evaluated stochastically
- $Q = \mathrm{Tr}\left\{\gamma_5 \mathbb{P}_M\right\}$ for chirally symmetric fermions
- spectral projectors are then also equivalent to the index (=stochastic way of counting the zero modes)
- for non-chirally symmetric fermions it still gives a clean definition, although chirality of modes is no longer $\pm 1 \longrightarrow \pm 1 + \mathcal{O}(a^2)$
- in practice, one evaluates the observable:
$$\mathcal{C} = \frac{1}{N} \sum_{k=1}^{N} \left(\mathbb{P}_M \eta_k, \gamma_5 \mathbb{P}_M \eta_k\right),$$
- uniqueness: dependence on the M of $\mathbb{P}_M$
- pros: theoretically clean, still rather cheap
- cons: stochastic ingredient, non-integer, Z_S/Z_P needed

Fermionic from disconnected loops

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- another fermionic definition, given by Chris Michael:

$$N_f Q = m_q \sum \bar{\psi}\gamma_5\psi = \sum \frac{m_q \gamma_5}{D + m_q},$$

  in the limit as $m_q \to 0$.
- allows for a Q computation as a by-product of evaluation of disconnected loops
- uniqueness: yes
- pros: cheap if treated as a by-product
- cons: unclear to what extent it is valid, stochastic ingredient, non-integer, Z_S/Z_P needed

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Field theoretic

- a very natural definition
- in the continuum:

$$Q = \frac{1}{32\pi^2} \int \mathrm{d}^4x \, \epsilon_{\mu\nu\rho\sigma} \mathrm{tr}[F_{\mu\nu}(x) F_{\rho\sigma}]$$

- on the lattice one has to choose some discretization
- renormalization:

$$q_R[U] = \mathrm{round}(Z q_{\mathrm{bare}}[U]),$$

Z is the (non-zero) solution of:

$$\min \sum_U (Z q_{\mathrm{bare}} - \mathrm{round}(Z q_{\mathrm{bare}}[U]))^2$$

- smoothing of gauge fields needed

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Field theoretic

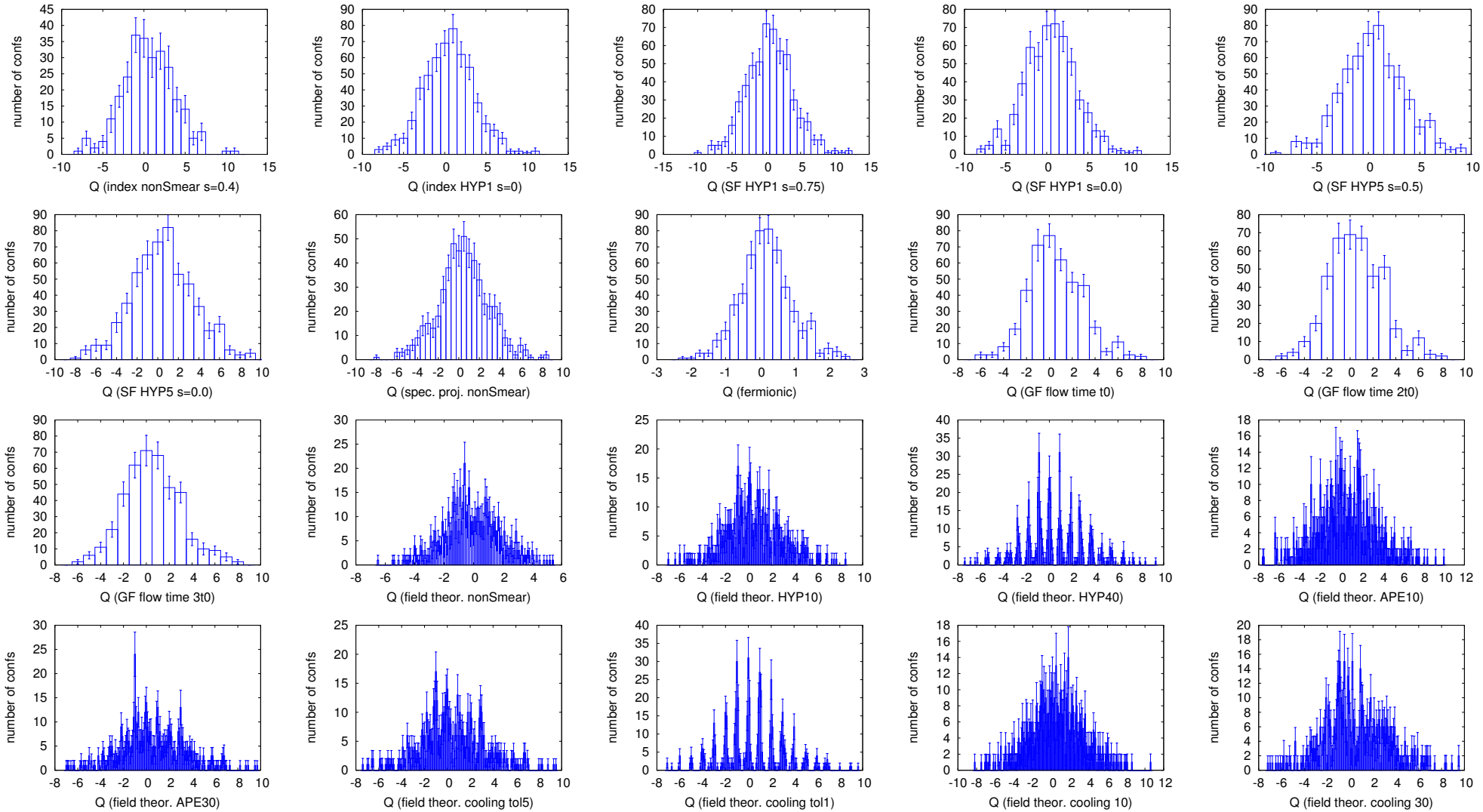
- smoothing:
  - ⋆ cooling – an iterative minimization of the lattice action, eliminates rough topological fluctuations while keeping large instantons unchanged and decreases renormalization effects by smoothing out the UV noise
    [B. Berg, 1981], [Y. Iwasaki et al., 1983], [M. Teper, 1985], [E. Ilgenfritz et al., 1986]
  - ⋆ HYP/APE smearing [M. Albanese et al., 1987], [A. Hasenfratz, F. Knechtli, 2001]
  - ⋆ gradient flow (GF) [M. Lüscher, 2010]
- GF is very important from the point of view of validity of the field theoretic approach
- uniqueness: discretization of F, level of smoothing
- pros: very cheap (but: cost of smoothing), theor. clean if GF used for smoothing and no renorm. then [M. Lüscher, P. Weisz, 2011]
- cons: HYP/APE or cooling a bit *ad hoc* (require renorm.)

Lattice setup

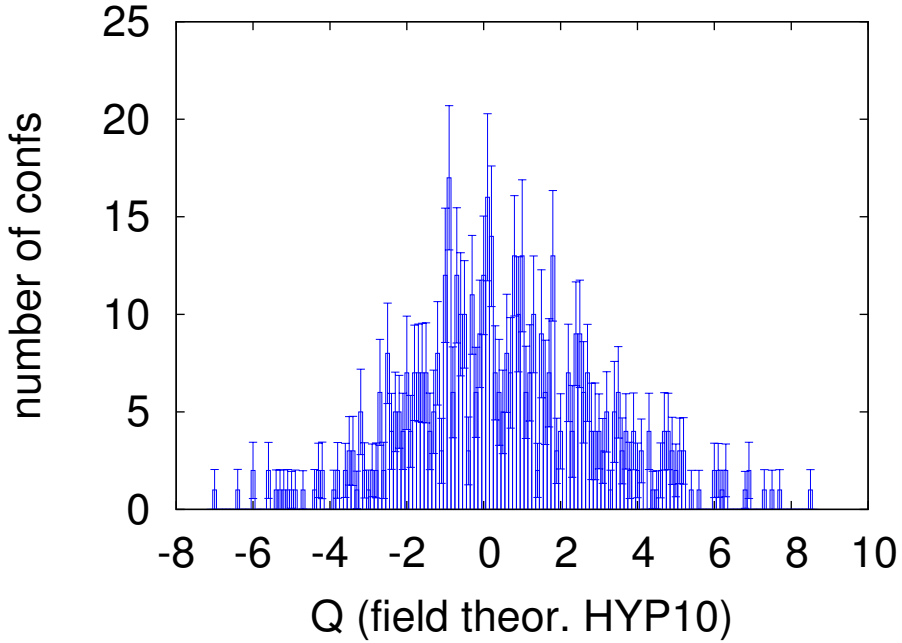
Ensemble	β	lattice	$a\mu_l$	μ_R [MeV]	κ_c	L [fm]	$m_\pi L$
b40.16	3.90	$16^3 \times 32$	0.004	21	0.160856	1.4	2.5
c30.20	4.05	$20^3 \times 40$	0.003	19	0.157010	1.3	2.4
d20.24	4.20	$24^3 \times 48$	0.002	15	0.154073	1.3	2.4
e17.32	4.35	$32^3 \times 64$	0.00175	16	0.151740	1.5	2.4

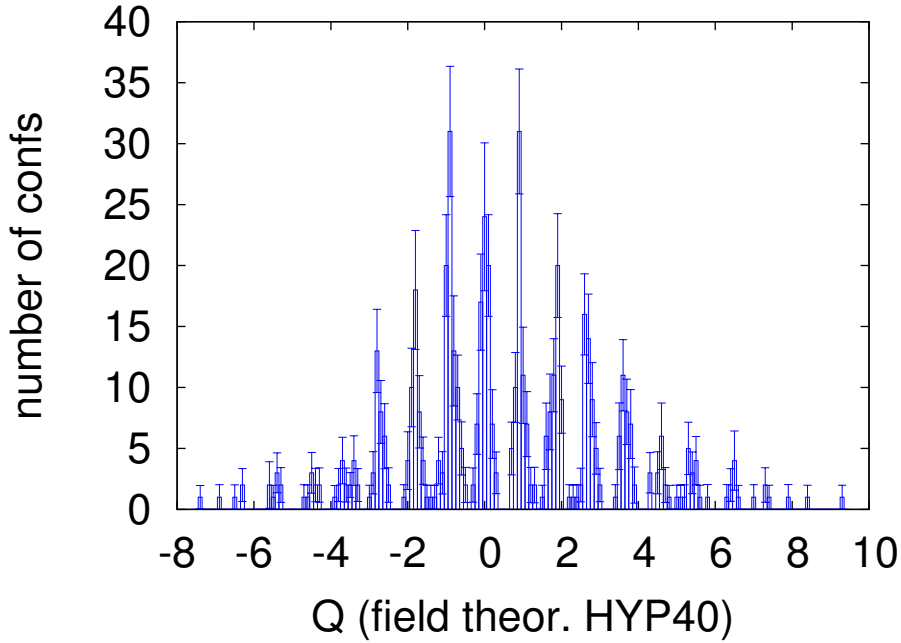
Ensemble	β	lattice	$a\mu_l$	$\mu_{l,R}$ [MeV]	κ_c	L [fm]	$m_\pi L$
A30.32	1.90	$32^3 \times 64$	0.0030	13	0.163272	2.8	4.0
A40.32	1.90	$32^3 \times 64$	0.0040	17	0.163270	2.8	4.5
A50.32	1.90	$32^3 \times 64$	0.0050	22	0.163267	2.8	5.1
A60.24	1.90	$24^3 \times 48$	0.0060	26	0.163265	2.1	4.2
A80.24	1.90	$24^3 \times 48$	0.0080	35	0.163260	2.1	4.8
B25.32	1.95	$32^3 \times 64$	0.0025	13	0.161240	2.5	3.4
B35.32	1.95	$32^3 \times 64$	0.0035	18	0.161240	2.5	4.0
B55.32	1.95	$32^3 \times 64$	0.0055	28	0.161236	2.5	5.0
B75.32	1.95	$32^3 \times 64$	0.0075	38	0.161232	2.5	5.8
B85.24	1.95	$24^3 \times 48$	0.0085	45	0.161231	1.9	4.7
D20.48	2.10	$48^3 \times 96$	0.0020	12	0.156357	2.9	3.9
D30.48	2.10	$48^3 \times 96$	0.0030	19	0.156355	2.9	4.7
D45.32	2.10	$32^3 \times 64$	0.0045	29	0.156315	1.9	3.9

Histograms – b40.16



Histograms – b40.16



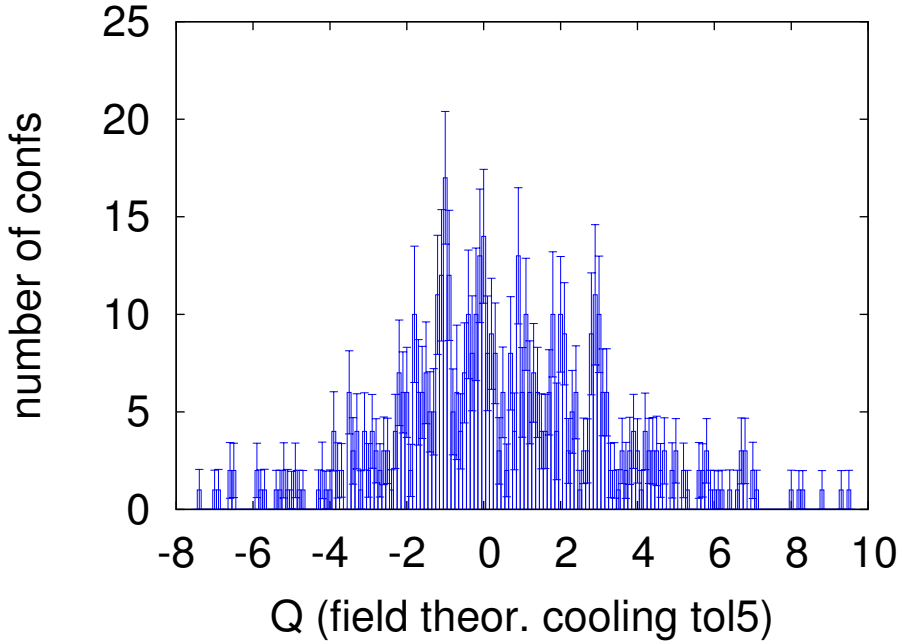


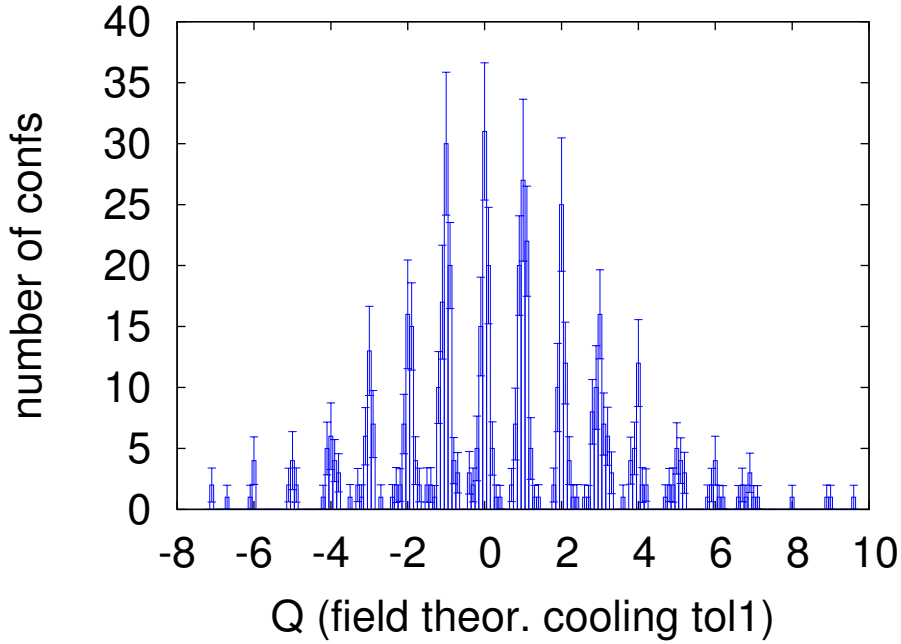
Field theoretic definition

10 HYP iterations

40 HYP iterations

Histograms – b40.16



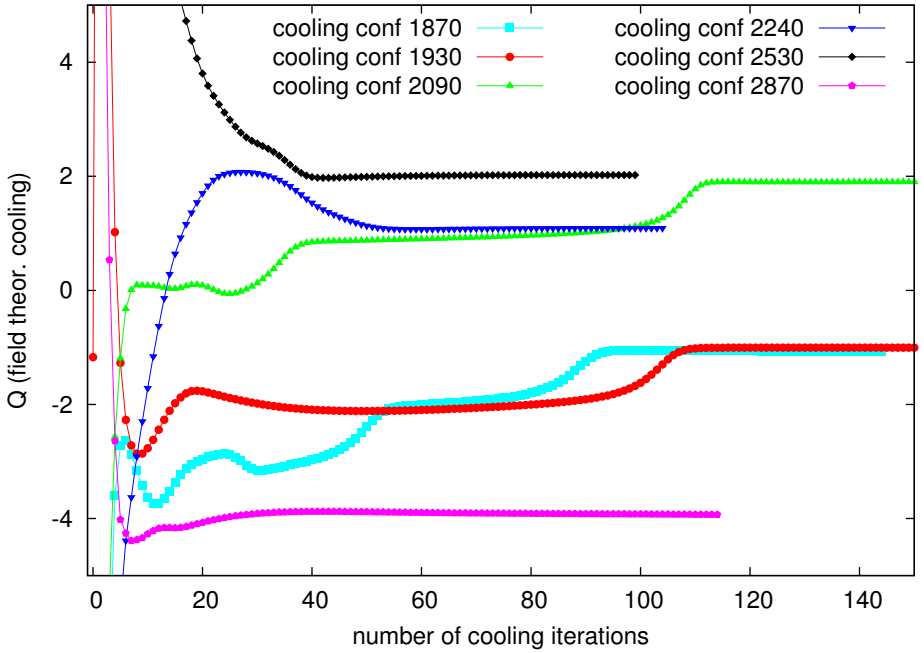


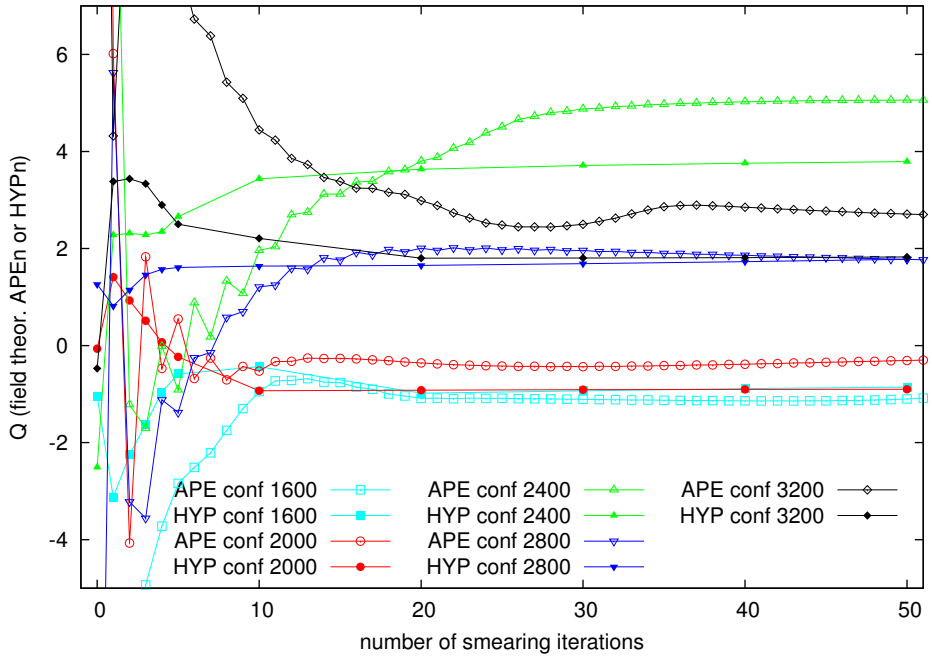
Field theoretic definition with cooling

5 steps with tol. 5%

10 steps with tol. 1%

Cooling vs. APE/HYP smearing



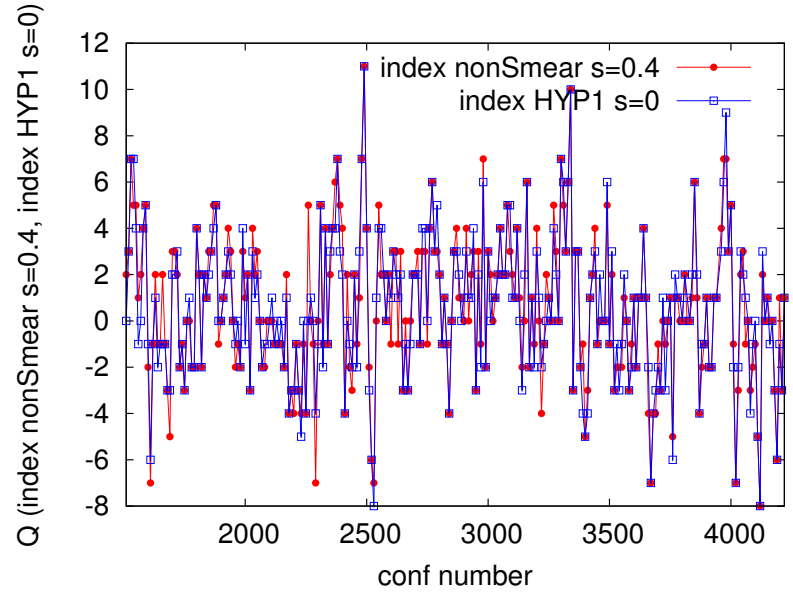


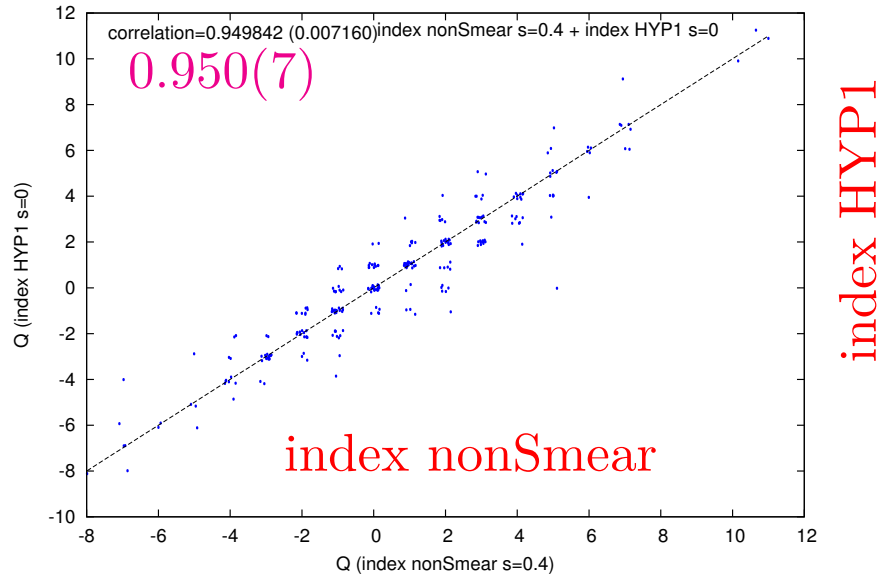
Field theoretic definition

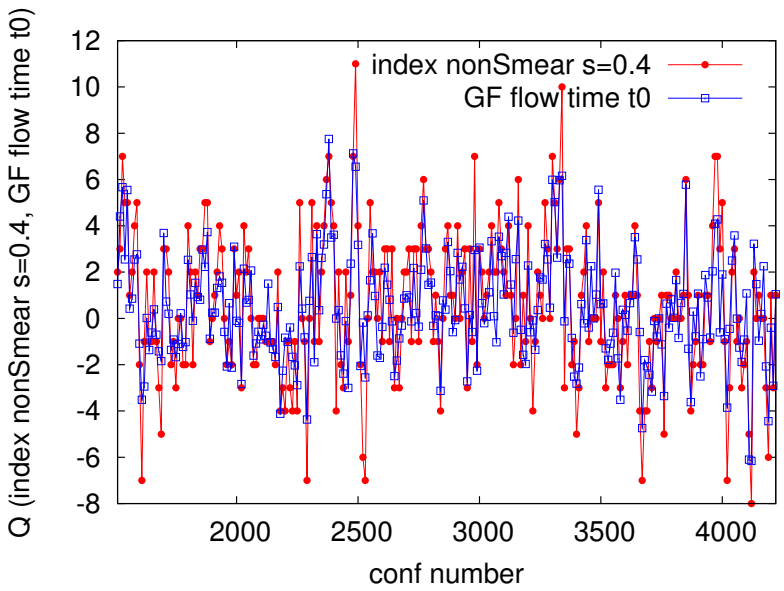
cooling

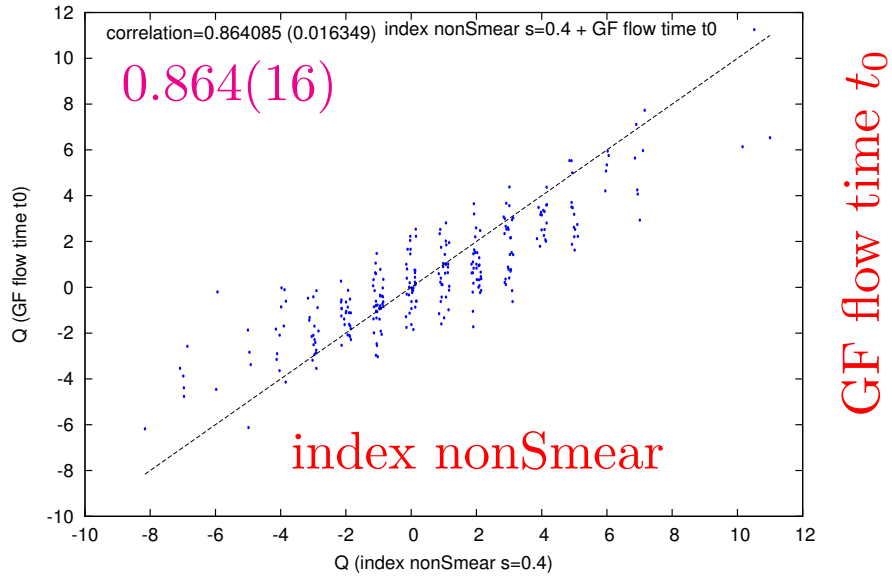
APE/HYP smearing

Pairwise comparisons









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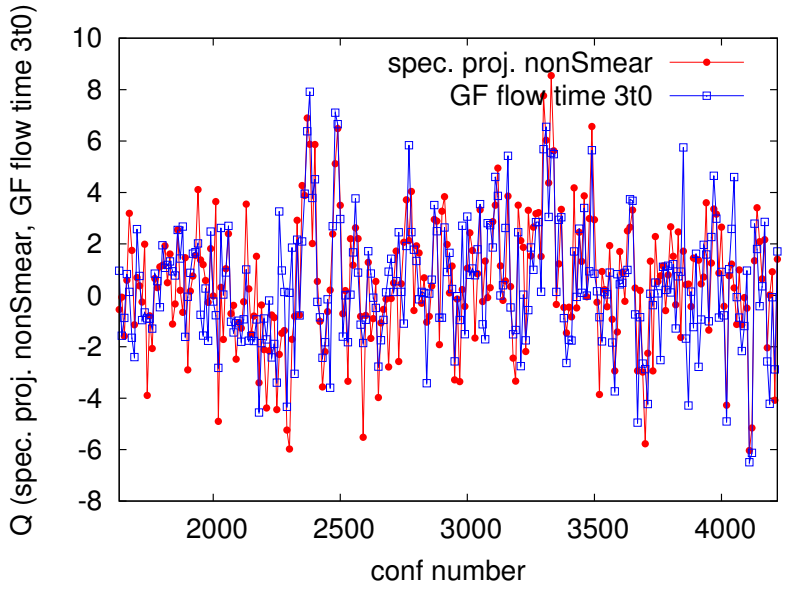

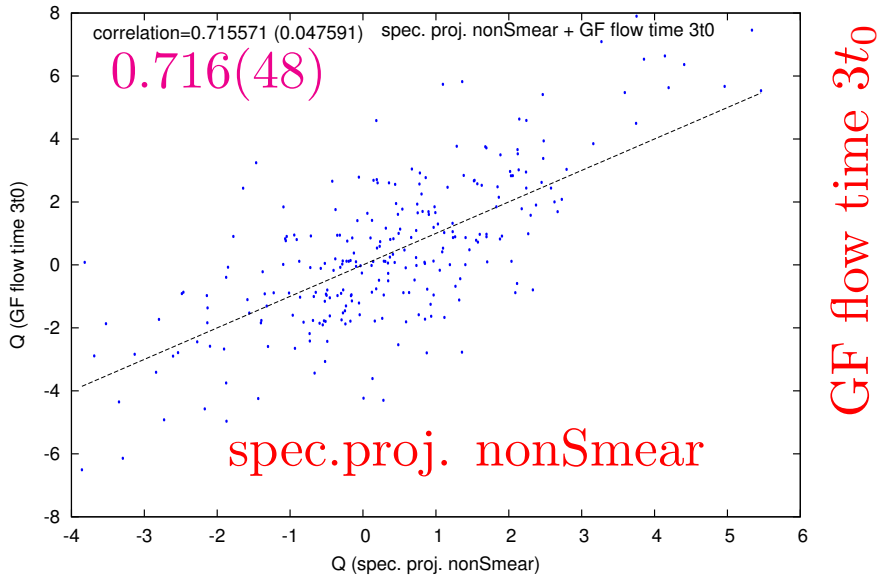

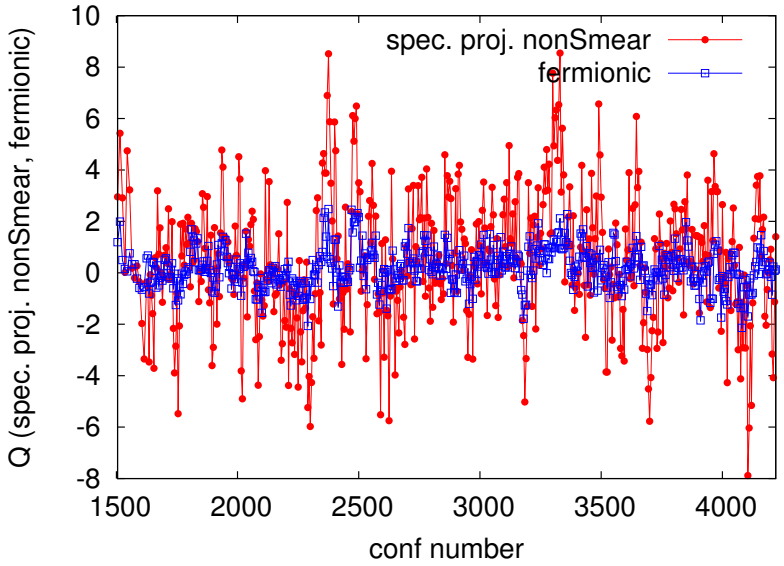

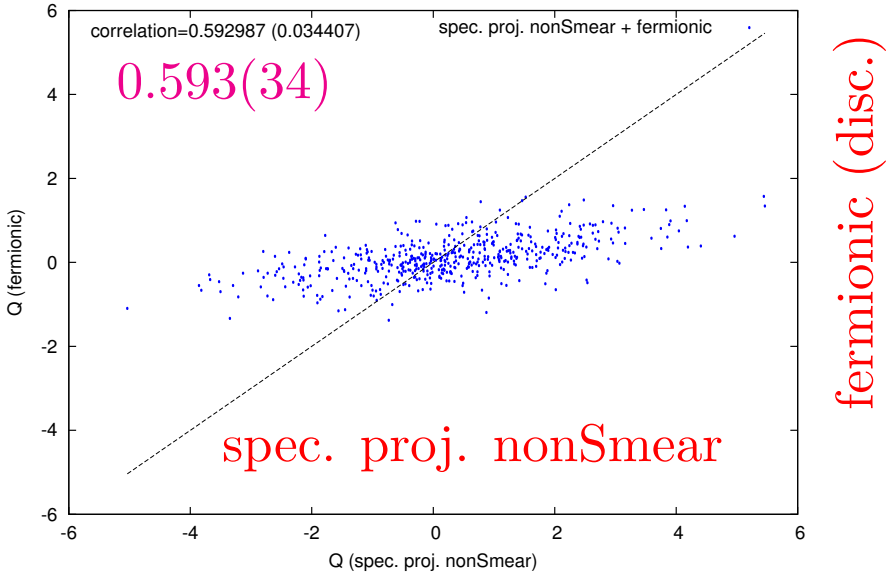

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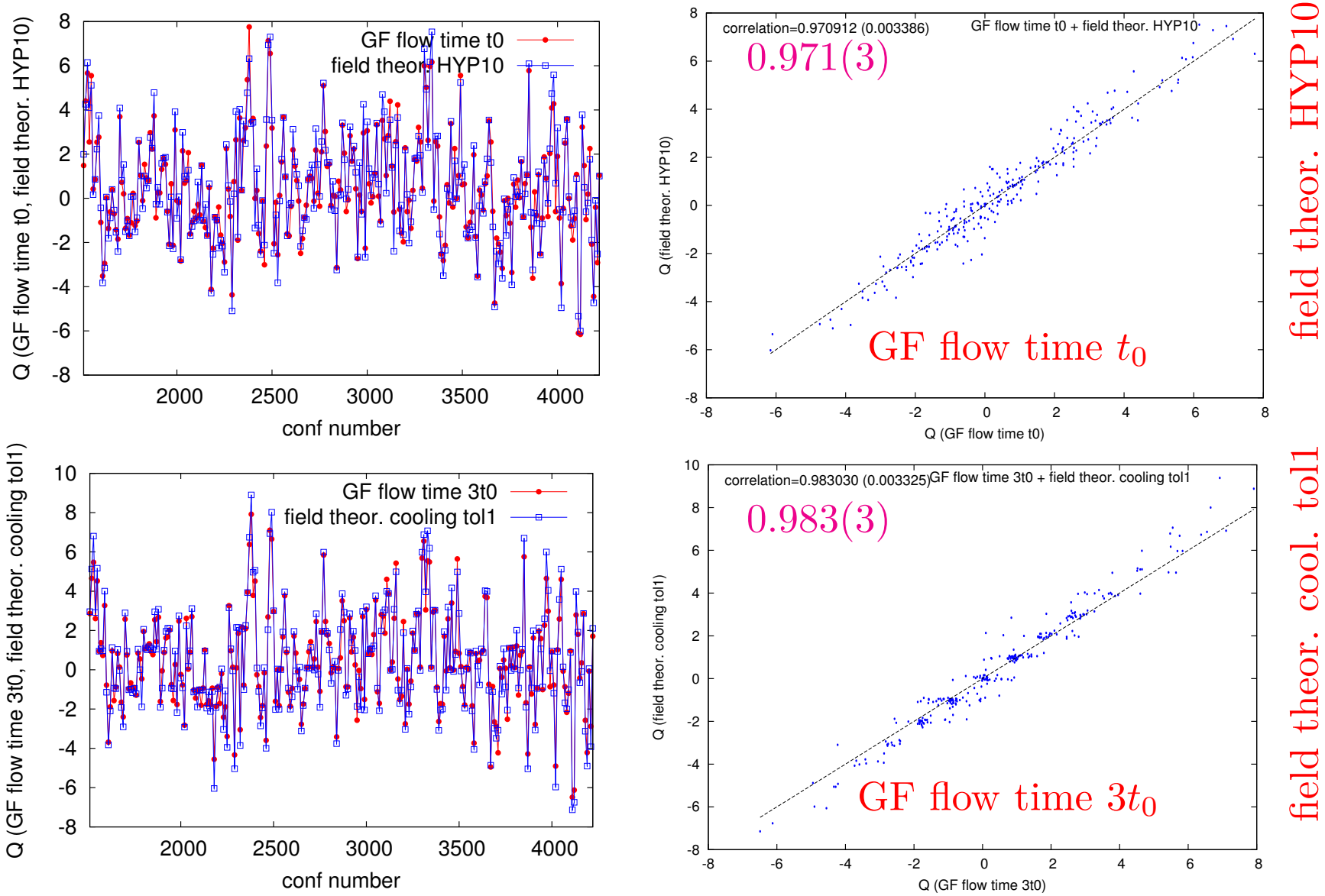
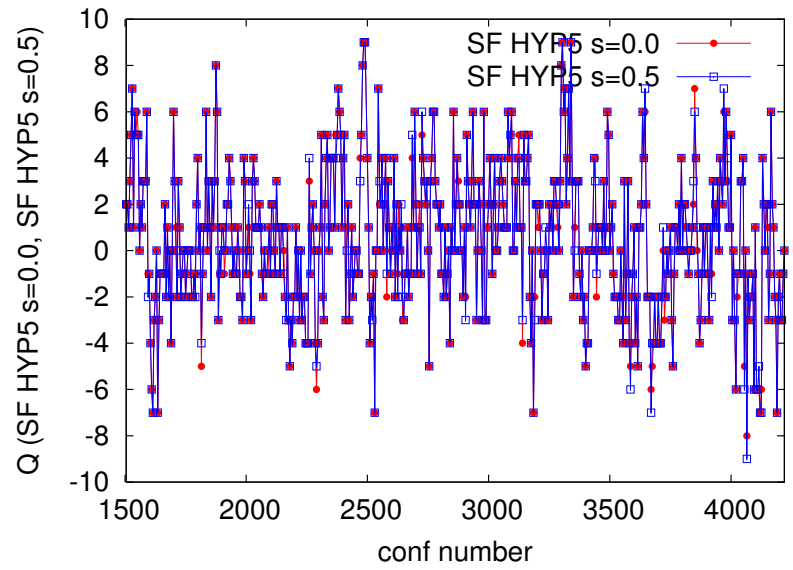
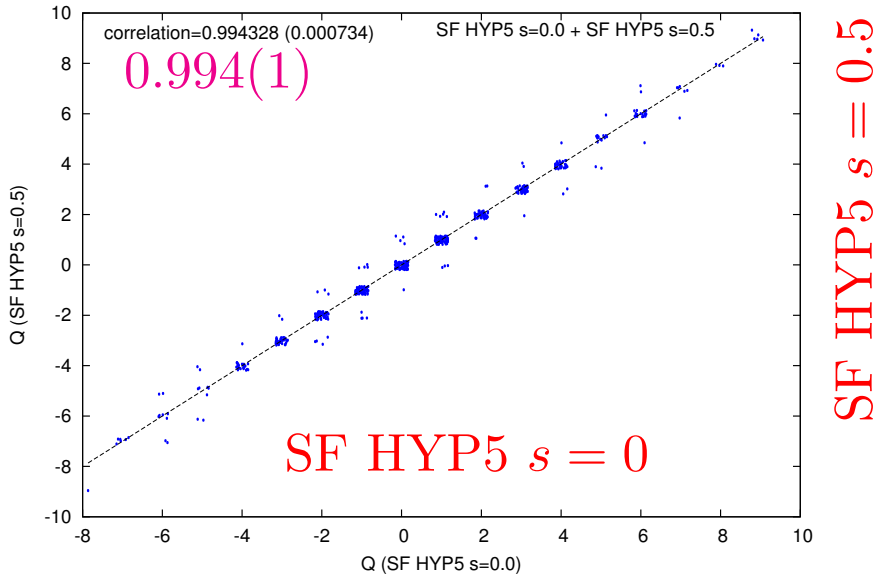
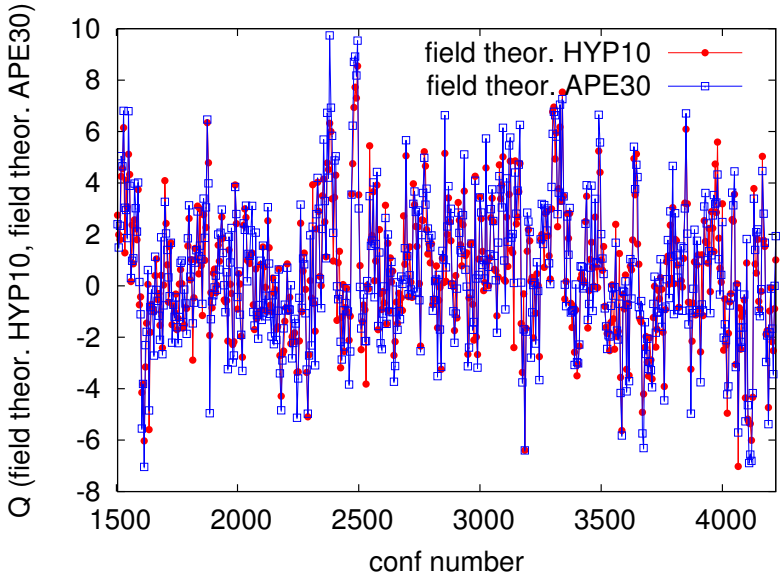
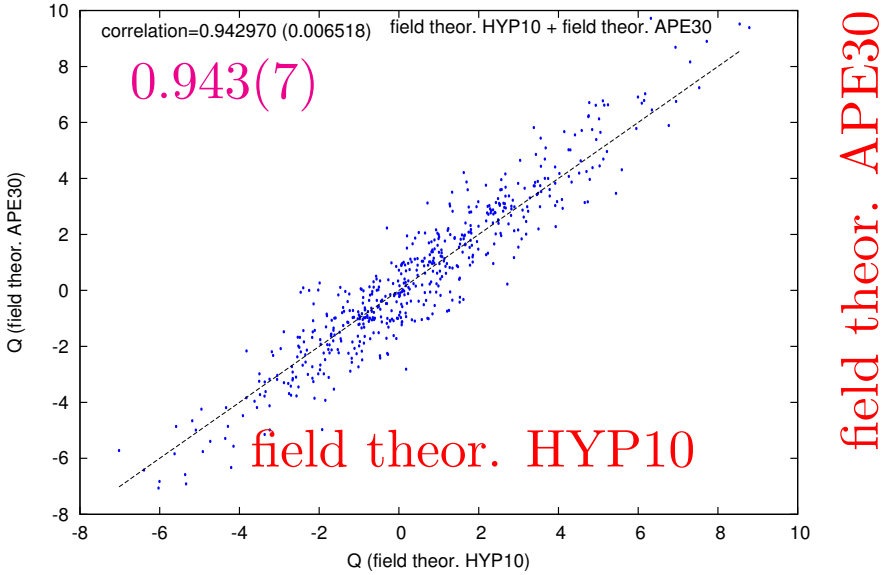


Pairwise comparisons









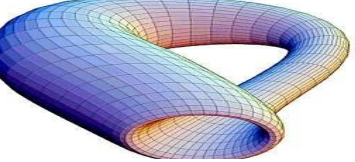


Table of correlations

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21
1	1.000(0)	0.889(12)	0.950(7)	0.877(15)	0.951(4)	0.929(9)	0.924(10)	0.585(51)	0.473(45)	0.864(16)	0.827(21)	0.814(20)	0.180(59)	0.907(12)	0.889(15)	0.909(10)	0.838(19)	0.830(20)	0.810(21)	0.889(12)	0.848(18)
2	0.889(12)	1.000(0)	0.903(10)	0.881(11)	0.901(10)	0.893(10)	0.888(11)	0.570(42)	0.489(45)	0.849(16)	0.807(22)	0.792(22)	0.208(40)	0.892(11)	0.874(13)	0.987(1)	0.850(16)	0.836(18)	0.795(21)	1.000(0)	0.867(14)
3	0.950(7)	0.903(10)	1.000(0)	0.898(10)	0.990(2)	0.937(6)	0.933(6)	0.553(43)	0.461(48)	0.864(16)	0.822(22)	0.806(23)	0.168(44)	0.924(8)	0.906(9)	0.923(9)	0.847(16)	0.837(18)	0.808(20)	0.903(10)	0.863(14)
4	0.877(15)	0.881(11)	0.898(10)	1.000(0)	0.907(9)	0.855(13)	0.847(13)	0.499(46)	0.395(50)	0.775(25)	0.733(31)	0.715(33)	0.184(41)	0.834(15)	0.811(17)	0.875(12)	0.770(21)	0.752(24)	0.725(25)	0.881(11)	0.782(21)
5	0.951(4)	0.901(10)	0.990(2)	0.907(9)	1.000(0)	0.935(6)	0.928(6)	0.549(42)	0.456(51)	0.865(15)	0.823(21)	0.808(22)	0.173(43)	0.919(8)	0.901(9)	0.920(8)	0.845(15)	0.836(16)	0.806(20)	0.901(10)	0.859(14)
6	0.929(9)	0.893(10)	0.937(6)	0.855(13)	0.935(6)	1.000(0)	0.994(0)	0.561(46)	0.455(44)	0.916(9)	0.867(16)	0.853(17)	0.155(45)	0.967(3)	0.944(5)	0.928(7)	0.882(12)	0.880(12)	0.834(15)	0.893(10)	0.898(10)
7	0.924(10)	0.888(11)	0.933(6)	0.847(13)	0.928(6)	0.994(0)	1.000(0)	0.561(48)	0.454(47)	0.923(8)	0.875(16)	0.860(17)	0.154(41)	0.972(2)	0.951(5)	0.926(8)	0.892(11)	0.890(11)	0.842(15)	0.888(11)	0.906(10)
8	0.585(51)	0.570(42)	0.553(43)	0.499(46)	0.549(42)	0.561(46)	0.561(48)	1.000(0)	0.593(34)	0.707(46)	0.716(44)	0.716(47)	0.093(39)	0.619(40)	0.608(41)	0.581(42)	0.619(38)	0.613(40)	0.649(36)	0.570(42)	0.613(40)
9	0.473(45)	0.489(45)	0.461(48)	0.395(50)	0.456(51)	0.455(44)	0.454(47)	0.593(34)	1.000(0)	0.545(44)	0.558(42)	0.566(38)	0.053(45)	0.516(47)	0.502(52)	0.501(46)	0.519(45)	0.510(44)	0.553(39)	0.489(45)	0.520(45)
10	0.864(16)	0.849(16)	0.864(16)	0.775(25)	0.865(15)	0.916(9)	0.923(8)	0.707(46)	0.545(44)	1.000(0)	0.976(3)	0.962(4)	0.152(56)	0.971(3)	0.967(4)	0.904(10)	0.981(3)	0.974(4)	0.954(6)	0.849(16)	0.988(1)
11	0.827(21)	0.807(22)	0.822(22)	0.733(31)	0.823(21)	0.867(16)	0.875(16)	0.716(44)	0.558(42)	0.976(3)	1.000(0)	0.992(1)	0.133(58)	0.934(9)	0.938(8)	0.859(16)	0.982(3)	0.966(6)	0.978(4)	0.807(22)	0.973(5)
12	0.814(20)	0.792(22)	0.806(23)	0.715(33)	0.808(22)	0.853(17)	0.860(17)	0.716(47)	0.566(38)	0.962(4)	0.992(1)	1.000(0)	0.139(57)	0.918(10)	0.922(9)	0.843(18)	0.964(6)	0.952(7)	0.983(3)	0.792(22)	0.955(7)
13	0.180(59)	0.208(40)	0.168(44)	0.184(41)	0.173(43)	0.155(45)	0.154(41)	0.093(39)	0.053(45)	0.152(56)	0.133(58)	0.139(57)	1.000(0)	0.168(45)	0.166(50)	0.200(42)	0.149(45)	0.175(47)	0.128(45)	0.208(40)	0.161(45)
14	0.907(12)	0.892(11)	0.924(8)	0.834(15)	0.919(8)	0.967(3)	0.972(2)	0.619(40)	0.516(47)	0.971(3)	0.934(9)	0.918(10)	0.168(45)	1.000(0)	0.987(1)	0.935(7)	0.943(6)	0.938(8)	0.903(11)	0.892(11)	0.954(5)
15	0.889(15)	0.874(13)	0.906(9)	0.811(17)	0.901(9)	0.944(5)	0.951(5)	0.608(41)	0.502(52)	0.967(4)	0.938(8)	0.922(9)	0.166(50)	0.987(1)	1.000(0)	0.919(9)	0.946(6)	0.941(7)	0.907(11)	0.874(13)	0.955(5)
16	0.909(10)	0.987(1)	0.923(9)	0.875(12)	0.920(8)	0.928(7)	0.926(8)	0.581(42)	0.501(46)	0.904(10)	0.859(16)	0.843(18)	0.200(42)	0.935(7)	0.919(9)	1.000(0)	0.897(11)	0.887(13)	0.840(18)	0.987(1)	0.915(9)
17	0.838(19)	0.850(16)	0.847(16)	0.770(21)	0.845(15)	0.882(12)	0.892(11)	0.619(38)	0.519(45)	0.981(3)	0.982(3)	0.964(6)	0.149(45)	0.943(6)	0.946(6)	0.897(11)	1.000(0)	0.979(3)	0.955(6)	0.850(16)	0.994(0)
18	0.830(20)	0.836(18)	0.837(18)	0.752(24)	0.836(16)	0.880(12)	0.890(11)	0.613(40)	0.510(44)	0.974(4)	0.966(6)	0.952(7)	0.175(47)	0.938(8)	0.941(7)	0.887(13)	0.979(3)	1.000(0)	0.939(8)	0.836(18)	0.979(4)
19	0.810(21)	0.795(21)	0.808(20)	0.725(25)	0.806(20)	0.834(15)	0.842(15)	0.649(36)	0.553(39)	0.954(6)	0.978(4)	0.983(3)	0.128(45)	0.903(11)	0.907(11)	0.840(18)	0.955(6)	0.939(8)	1.000(0)	0.795(21)	0.942(7)
20	0.889(12)	1.000(0)	0.903(10)	0.881(11)	0.901(10)	0.893(10)	0.888(11)	0.570(42)	0.489(45)	0.849(16)	0.807(22)	0.792(22)	0.208(40)	0.892(11)	0.874(13)	0.987(1)	0.850(16)	0.836(18)	0.795(21)	1.000(0)	0.867(14)
21	0.848(18)	0.867(14)	0.863(14)	0.782(21)	0.859(14)	0.898(10)	0.906(10)	0.613(40)	0.520(45)	0.988(1)	0.973(5)	0.955(7)	0.161(45)	0.954(5)	0.955(5)	0.915(9)	0.994(0)	0.979(4)	0.942(7)	0.867(14)	1.000(0)

1 = index nonSmear $s = 0.4$, 2 = index nonSmear $s = 0$, 3 = index HYP1 $s = 0$,
4 = SF HYP1 $s = 0.75$, 5 = SF HYP1 $s = 0$, 6 = SF HYP5 $s = 0.5$, 7 = SF HYP5 $s = 0$,
8 = spec.proj. nonSmear, 9 = fermionic (from disc. loops),
10 = GF flow time t_0, 11 = GF flow time $2t_0$, 12 = GF flow time $3t_0$,
13 = field theor. nonSmear, 14 = field. theor. HYP10, 15 = field. theor. HYP40,
16 = field. theor. APE10, 17 = field. theor. APE30, 18 = field theor.cool. tol. 5%,
19 = field theor. cool.tol. 1%, 20 = field theor. cool.10 steps, 21 = field theor.cool. 30 steps

Plot of correlations

Presentation outline

Introduction

Results

Histograms

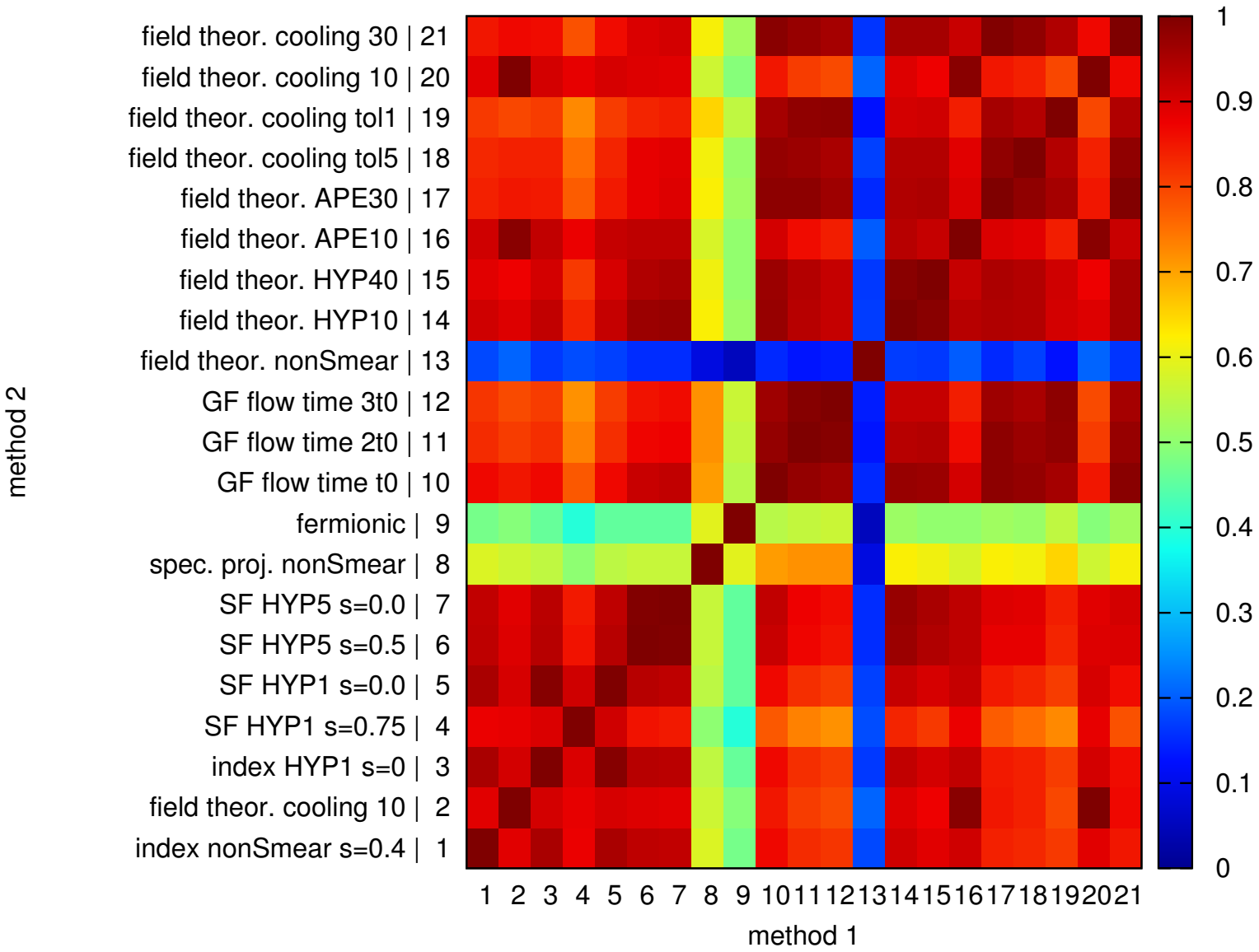
Cool. vs. APE/HYP

Pair comparisons

Correlations

Topo. susc.

Conclusions



Correlation towards the continuum limit

Presentation outline
Introduction
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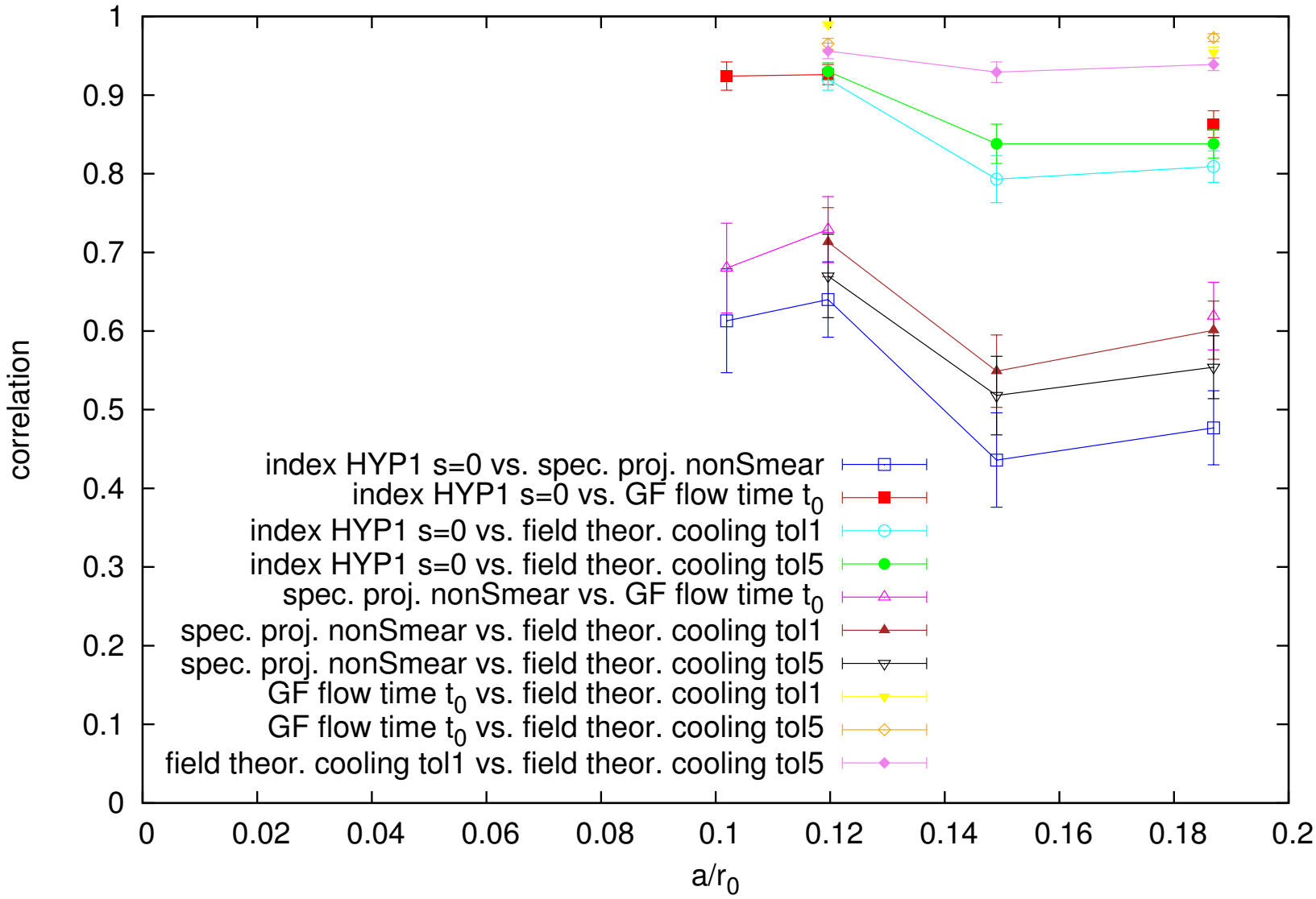
Histograms
Cool. vs. APE/HYP
Pair comparisons
Correlations
Topo. susc.
Conclusions



Topological susceptibility – b40.16

Presentation outline
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Pair comparisons
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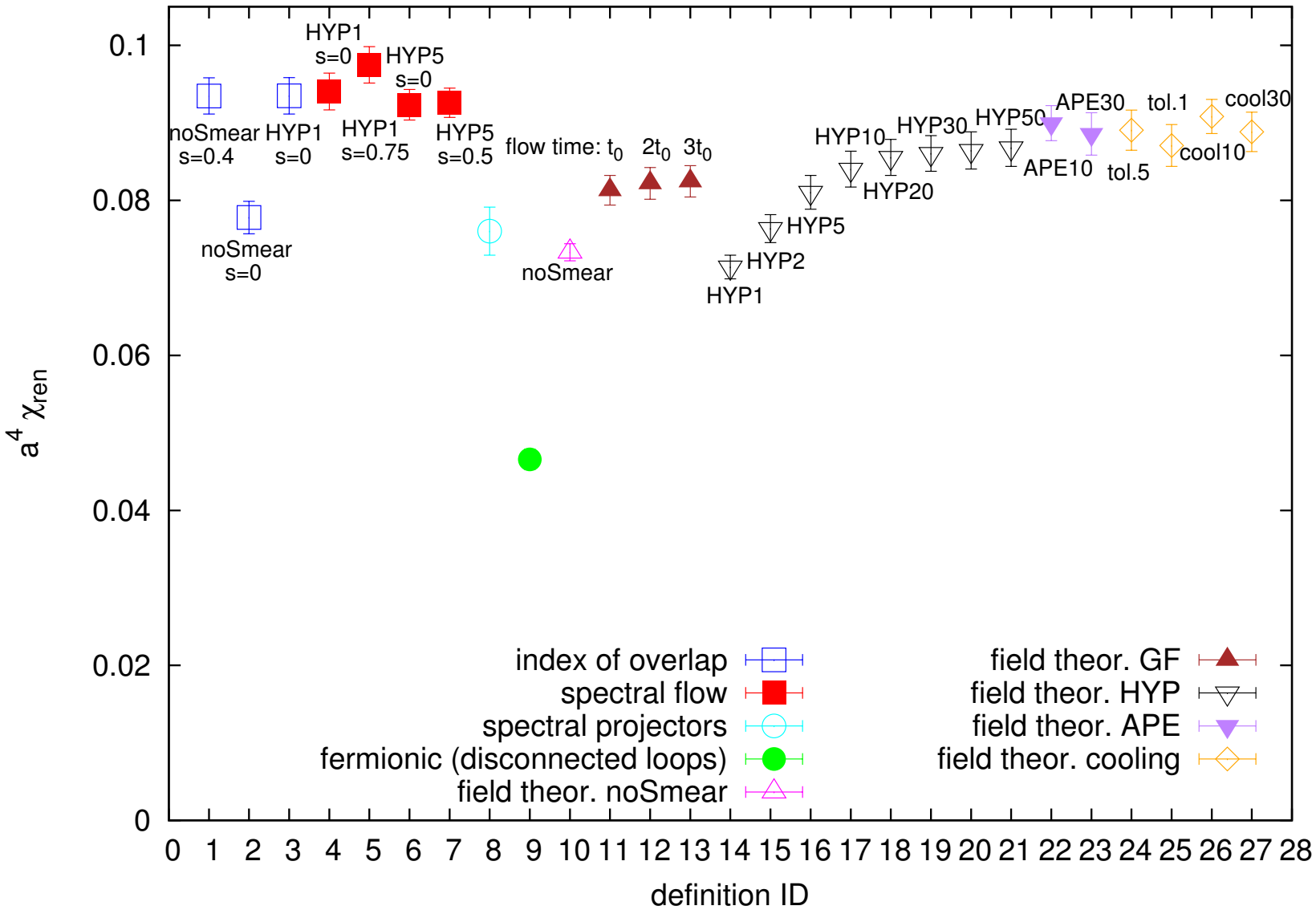
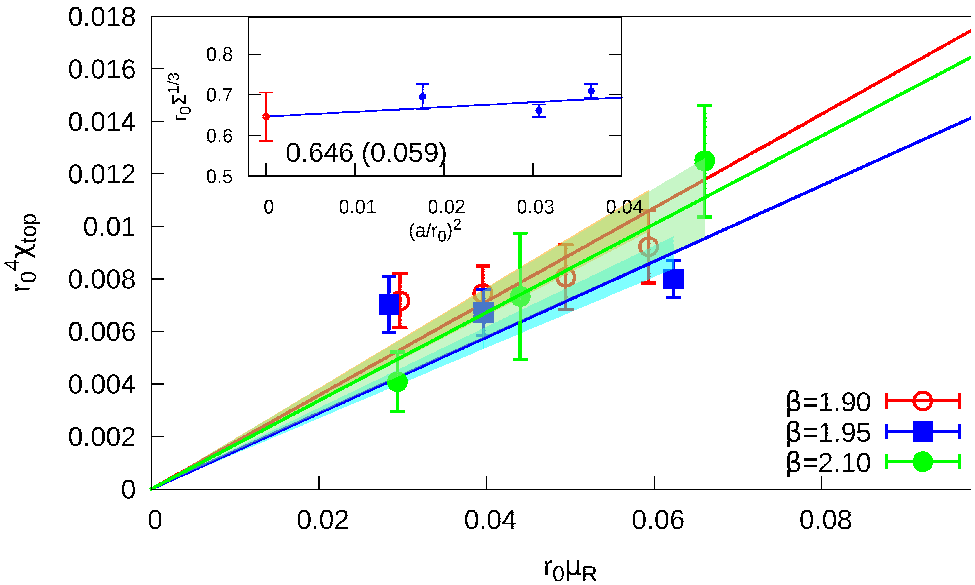
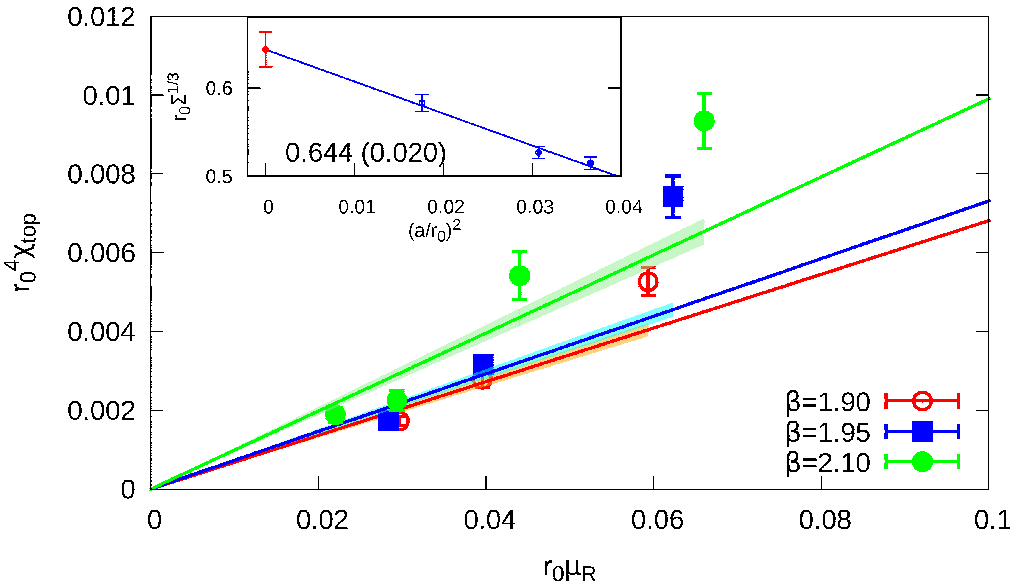
Topo. susc.
Conclusions



Topological susceptibility

used only pion masses $m_\pi \leq 400$ MeV





spectral projectors: $r_0\Sigma^{1/3} = 0.646(59)$ fermionic: $r_0\Sigma^{1/3} = 0.644(20)$

Tree-level χPT fit: $r_0^4\chi = \frac{r_0^3\Sigma \cdot r_0\mu_R}{2}$

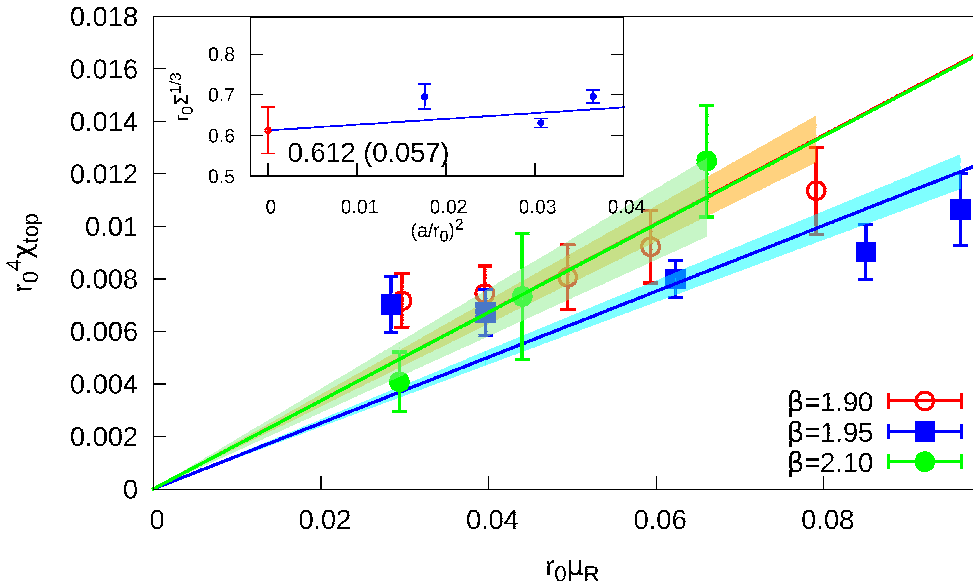
compare to direct determination

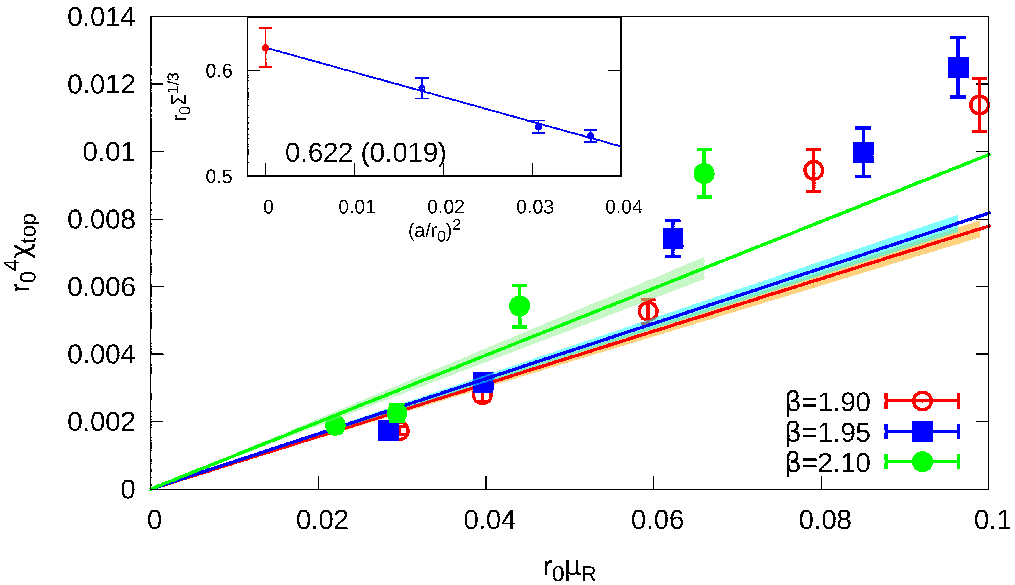
[K.C., E. García Ramos, K. Jansen, JHEP 10(2013)175]

$$r_0\Sigma^{1/3}_{cont,N_f=2+1+1} = 0.680(29)$$

Topological susceptibility

used all pion masses ($m_\pi = [260, 500]$ MeV)





spectral projectors: $r_0\Sigma^{1/3} = 0.612(57)$ fermionic: $r_0\Sigma^{1/3} = 0.622(19)$

Tree-level χPT fit: $r_0^4\chi = \frac{r_0^3\Sigma\cdot r_0\mu_R}{2}$

compare to direct determination

[K.C., E. García Ramos, K. Jansen, JHEP 10(2013)175]

$$r_0\Sigma^{1/3}_{cont,N_f=2+1+1} = 0.680(29)$$

My subjective ranking of theoretical cleanness

From the cleanest to the problematic ones:

1. index of the overlap Dirac operator
   spectral flow
   field theoretic with gradient flow
   spectral projectors
2. field theoretic with smearing
3. field theoretic with cooling
4. fermionic from disconnected loops

The theoretical progress of recent years (spectral projectors, gradient flow) makes the non-clean definitions rather unattractive – there is basically no need any more to use them for reasons of (relatively small) computational intensity.

Conclusions

- There are many definitions of the topological charge on the lattice
- No clear answer which definition to use
- We observe high correlations between different definitions...
- ...and these correlations seem to increase towards the continuum limit
- Perhaps the best compromise between theoretical cleanness and computational cost: field theoretic with gradient flow

[M. Bruno, S. Schaefer, R. Sommer, arXiv:1406.5363 [hep-lat]]

Thank you for attention!