Solving $\mathrm{SU}(3)$ Yang-Mills theory on the lattice: a calculation of selected gauge observables with gradient flow

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04.07.19

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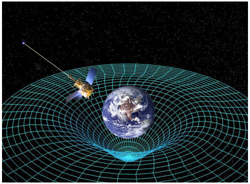
Co-supervisor: *Morten Hjorth-Jensen*

University of Oslo

The four forces of nature



Gravity

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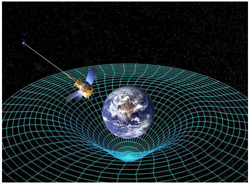

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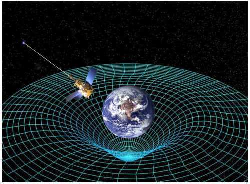

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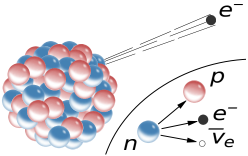

Weak nuclear force

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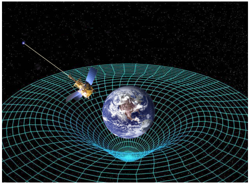

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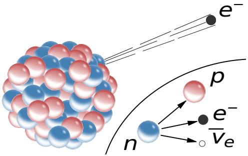

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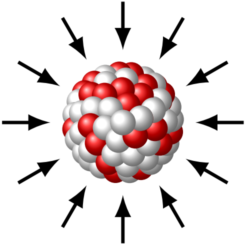

Strong nuclear force

What is the strong force?

Consists of:

- 6 quark flavors: up, down, strange, charm, bottom and top

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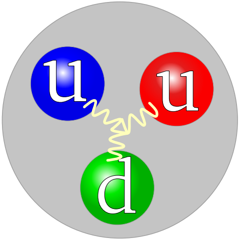

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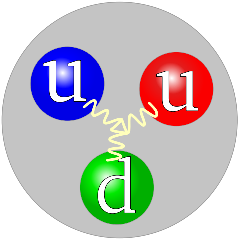
Mass discrepancy:

$$m_p \neq m_u + m_u + m_d,$$

936 MeV $\neq 3$ MeV $+ 3$ MeV $+ 6$ MeV.



Comparing the strong force and QED

Electromagnetism or Quantum Electrodynamics(QED), a U(1) symmetry theory:

$$\mathcal{L}_{\mathrm{QED}} = \sum_{f=\text{fermions}} \bar{\psi}_f (i\gamma^\mu(\partial_\mu + ieQ_f A_\mu) - m_f)\psi_f - \frac{1}{4} F_{\mu\nu}F^{\mu\nu}$$

Field strength tensor:

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The strong nuclear force or Quantum Chromo Dynamics(QCD), a $\mathrm{SU}(3)$ symmetry theory:

$$\mathcal{L}_{\mathrm{QCD}} = \sum_{f=u,d,\ldots} \bar{\psi}_f(i\gamma^\mu(\partial_\mu + ig_S A^a_\mu T^a) - m_f)\psi_f - \frac{1}{4}G^a_{\mu\nu}G^{a\mu\nu}$$

Field strength tensor:

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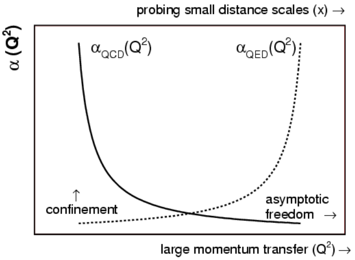

https://www-cdf.fnal.gov/~group/WORK/DISS_PAGE/diss_page.htm

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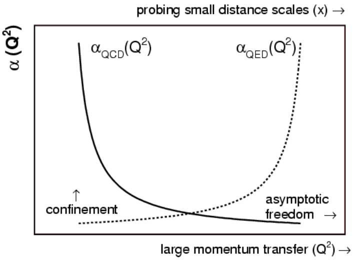

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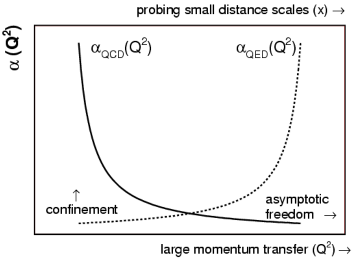

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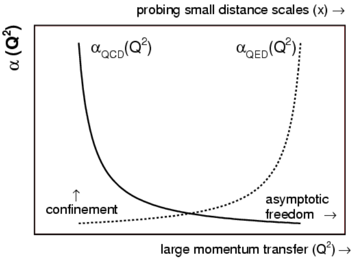

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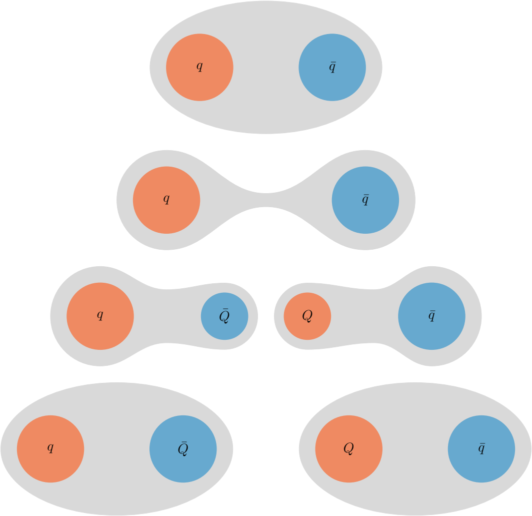
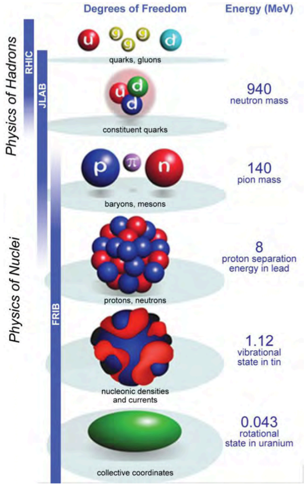
- Coupling constant α is the strength of the force in an interaction.
- QED becomes stronger - QCD becomes weaker at higher energies.
- Can't use perturbation theory on strong force in low-energy regime!
- Need to understand the low-energy regime to understand phenomenas such as **confinement**.

Confinement: a low-energy phenomena

No free quarks in nature!



QCD and nuclear physics



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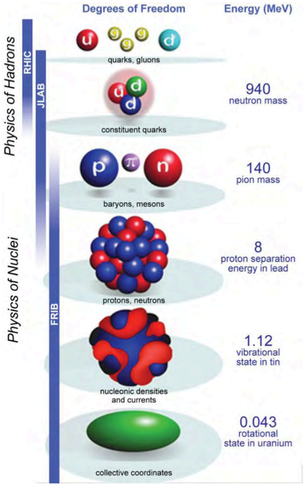

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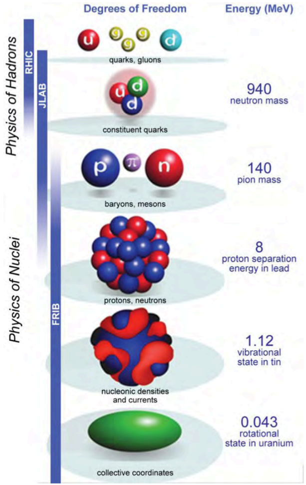

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- Need to understand the low-energy regime in order to better understand nuclear physics!
- Want to bridge the gap between theories that operate at different scales.
- $\rightarrow$ numerical methods(e.g. lattice QCD)

We currently have...

- A theory for QCD in the **continuum**.

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- $\rightarrow$ need to **discretize** the path integral.

But first, we need to know *what* a path integral is.

How we measure: path integrals

Going from t_0 at A to a time t_1 at B can be given in terms of a path integral.

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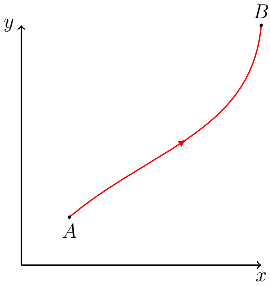

Classically, only one possible path obtained from the principle of least action.

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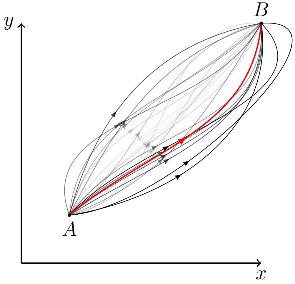

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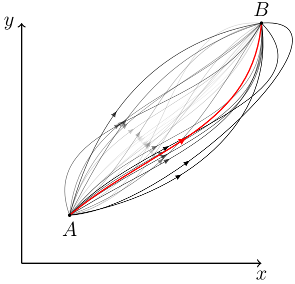

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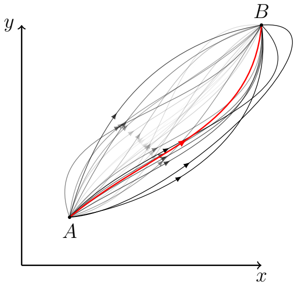

In quantum mechanics, there is lots of possible paths.
Principle of least action (or stationary condition): $\frac{\delta}{\delta x(t)}\left(S\left[x(t)\right]\right) = 0$
Sum over all possible paths $\rightarrow$ *the most likely path.*

Path integrals

Given a field ϕ_M in Minkowski space, the *partition function* Z is given by

$$
\begin{aligned}
Z &= \int \mathcal{D}\phi_M \mathrm{e}^{\frac{i}{\hbar} S_M[\phi_M]} \\
&\downarrow \quad \hbar = 1, \quad \tau \to -it \qquad \text{imaginary time}(\to \text{Euclidean space})! \\
&= \int \mathcal{D}\phi \mathrm{e}^{-S[\phi]}
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where $\mathcal{D}$ is an integration of all possible paths in space.

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An observable O becomes,

$$\langle O \rangle = \frac{1}{Z} \int \mathcal{D}\phi O[\phi] \mathrm{e}^{-S[\phi]}$$

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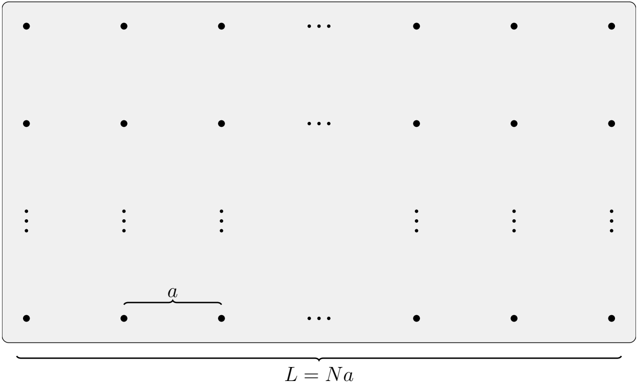
Difficult to calculate the all possible paths $\to$ discretize spacetime

Discretizing the path integral



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A **statistical approach** using importance sampling is needed for generating gauge configurations.

Configurations: comparing QCD and the Ising model

The 2D Ising model is given by:

$$H = -J \sum_{\langle i,j \rangle} S_i S_j - h \sum_i S_i$$

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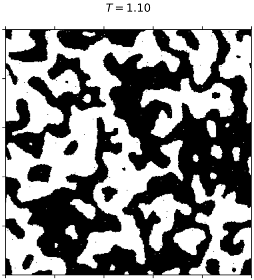
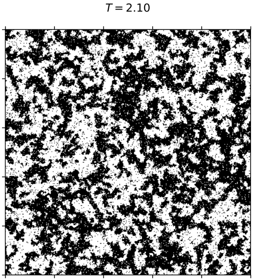
- A lattice in LQCD is however $N^4 = 10000$.

Then what is a configuration?

Looking at a spin lattice of the Ising model,





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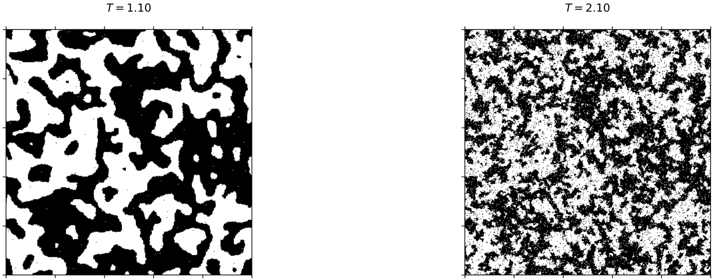

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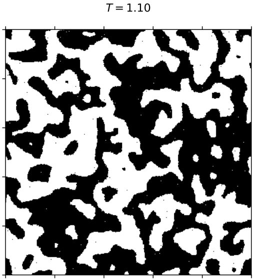
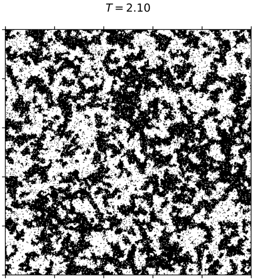




- A **configuration** in the Ising model is a given *arrangement of the spins*.
- A **configuration** in LQCD is a given *arrangement of the gauge field*.

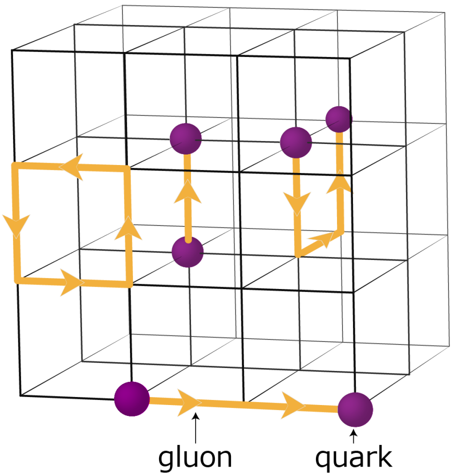
Sampling configurations

An expectation value becomes

$$\langle O \rangle = \frac{1}{N_{\text{cfg}}} \sum_{i=1}^{N_{\text{cfg}}} O[\phi_i] + \mathcal{O}\left(\frac{1}{\sqrt{N_{\text{cfg}}}}\right)$$

where ϕ_i is a generated gauge configuration(or just a general configuration).

QCD on the lattice



http://www.jicfus.jp/en/wp-content/uploads/2012/12/LatticeQCD.png

From QCD to pure $\mathrm{SU}(3)$ Yang-Mills

We exclude fermions to only look at the gauge fields,

$$S_G = \frac{1}{2} \int \mathrm{d}^4 x \mathrm{tr} \left(G_{\mu\nu} \right)^2$$

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From this we can build a lattice action,

$$S_G[U] = \frac{\beta}{3} \sum_{n\in\Lambda} \sum_{\mu<\nu} \mathrm{Re}\,\mathrm{tr}\left[1 - U_\mu(n)\, U_\nu(n+\hat{\mu})\, U_\mu(n+\hat{\nu})^\dagger\, U_\nu(n)^\dagger\right],$$

with $\beta = 6/g_S^2$

Parallelization: distributing the problem

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Number of points in a lattice:

$$\underbrace{N^3}_{\text{Spatial}} \times \underbrace{N_T}_{\text{Temporal}} \times \underbrace{4}_{\text{Links}} \times \underbrace{9}_{\mathrm{SU}(3)\text{ matrix}} \times \underbrace{2}_{\mathbb{C}\text{-numbers}} = 72N^3N_T,$$

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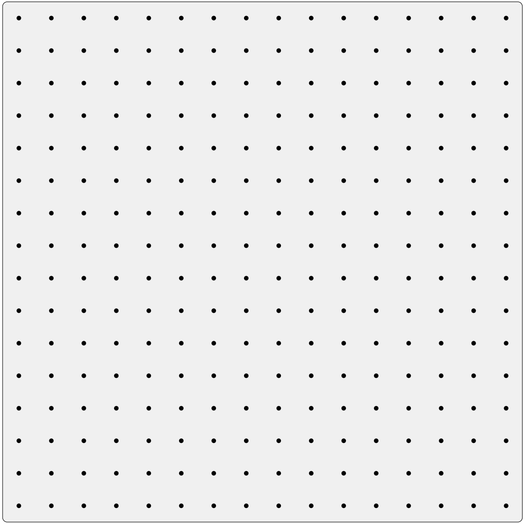
Too large to solve on any single computer.

Parallelization: splitting the hypercube



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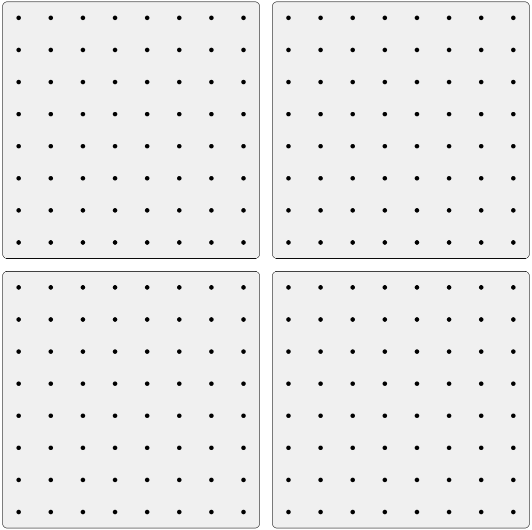

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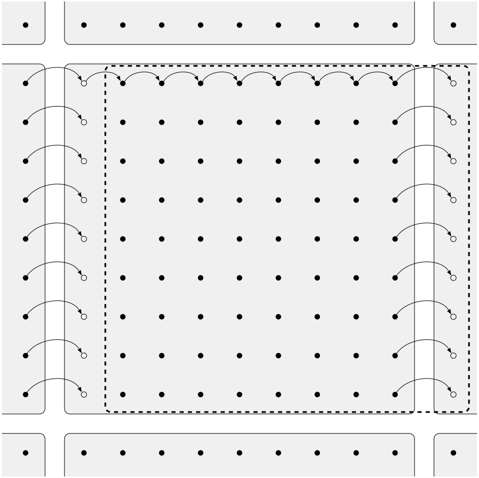

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However, some observable are problematic...

Gradient flow

$$\partial_{t_f} B_\mu(x, t_f) = D_\nu G_{\nu\mu}(x, t_f)$$
$$B_\mu(x, t_f)\Big|_{t_f=0} = A_\mu(x)$$

- Solves this by integrating along t_f called *flow time* [1]

[1] Lüscher [2010]

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$$B_\mu(x, t_f)\Big|_{t_f=0} = A_\mu(x)$$

- Solves this by integrating along t_f called *flow time* [1]
- $B_\mu(x, t_f)$ is the gauge field $A_\mu(x)$ at a flow time t_f.

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Gradient flow

$$
\begin{aligned}
\partial_{t_f} B_\mu(x, t_f) &= D_\nu G_{\nu\mu}(x, t_f) \\
B_\mu(x, t_f)\big|_{t_f=0} &= A_\mu(x)
\end{aligned}
$$

- Solves this by integrating along t_f called *flow time* [1]
- $B_\mu(x, t_f)$ is the gauge field $A_\mu(x)$ at a flow time t_f.
- $D_\nu = \partial_\nu + [B_\mu(x, t_f), \cdot]$

[1] Lüscher [2010]

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An analogy: the diffusion equation:

$$\frac{\partial}{\partial t_f} B_\mu(x, t_f) \approx \partial_x^2 B_\mu(x, t_f)$$

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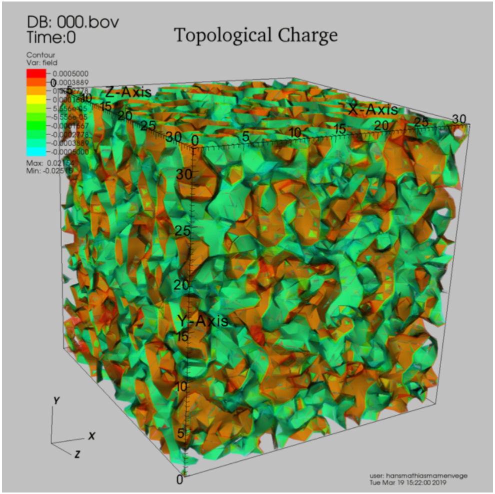
Gradient flow III: topological charge



Animation created using LatViz.

Results

Ensembles

Points in lattice given by $N^3 \times N_T$.

Ensemble	$\beta = 6/g_S^2$	N	N_T	N_{cfg}	a [fm]	Config. size[GB]
A	6.0	24	48	1000	$0.0931(4)$	0.356
B	6.1	28	56	1000	$0.0791(3)$	0.659
C	6.2	32	64	2000	$0.0679(3)$	1.125
D_1	6.45	32	32	1000	$0.0478(3)$	0.563
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A scale t_0 was set using the energy and gradient flow.

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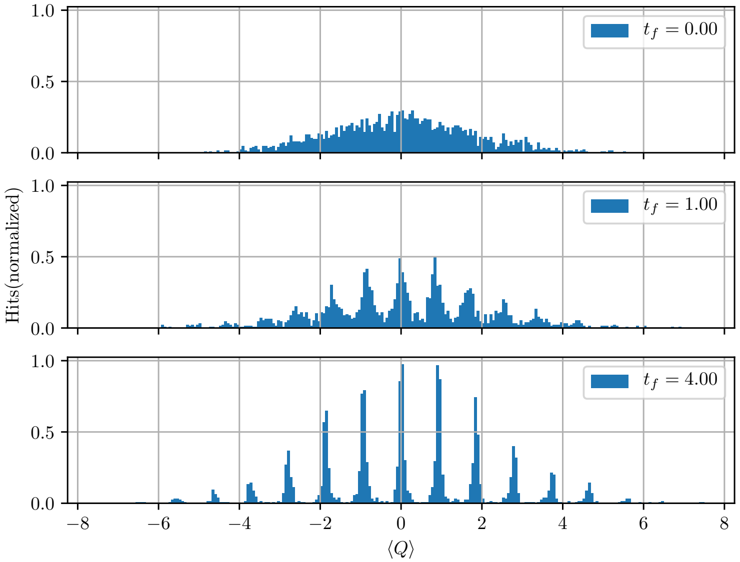
Integer valued and equally probably to have negative charge as positive,

$$\langle Q \rangle = 0$$

Topological charge distribution



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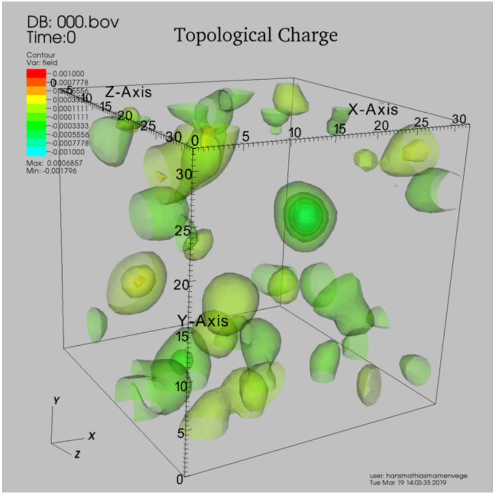
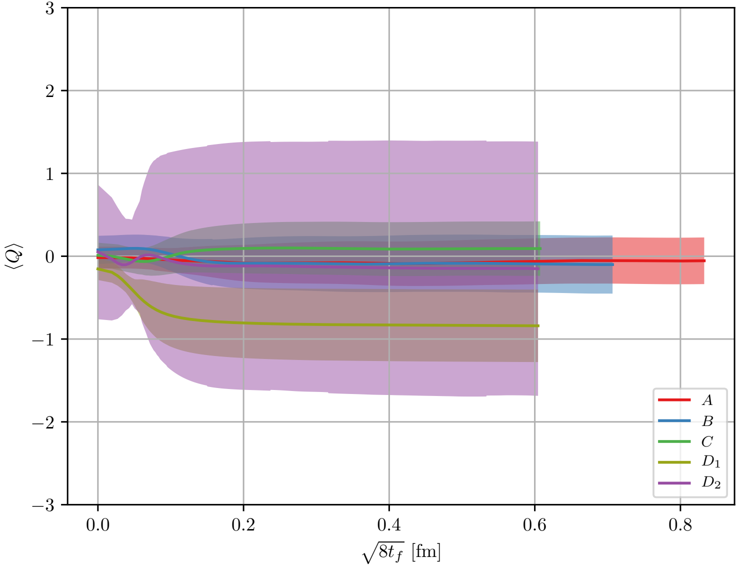


Animation created using LatViz.

Topological charge for our main ensembles



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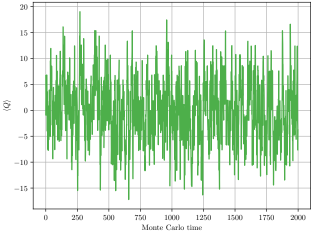
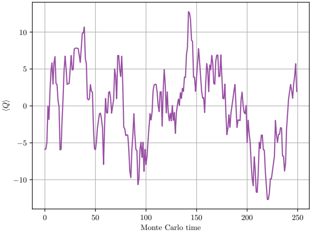
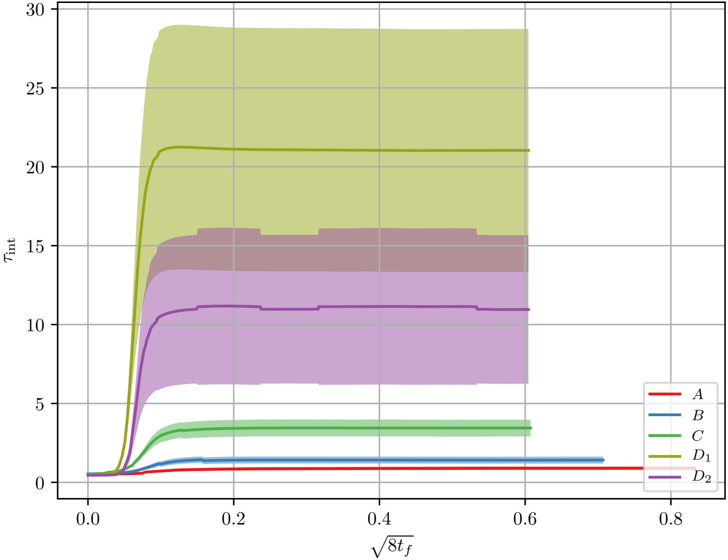


Ensemble C, $32^3 \times 64$, $\beta = 6.2$



Ensemble D_2, $48^3 \times 96$, $\beta = 6.45$

Topological charge autocorrelation



Critical slowing down

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- $\to$ many more lattice updates are required in order to have independent gauge configurations.

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$$\chi_{\mathrm{top}}^{1/4} = \frac{1}{V^{1/4}} \left\langle Q^2 \right\rangle^{1/4}$$

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We expect $N_f = 3$.

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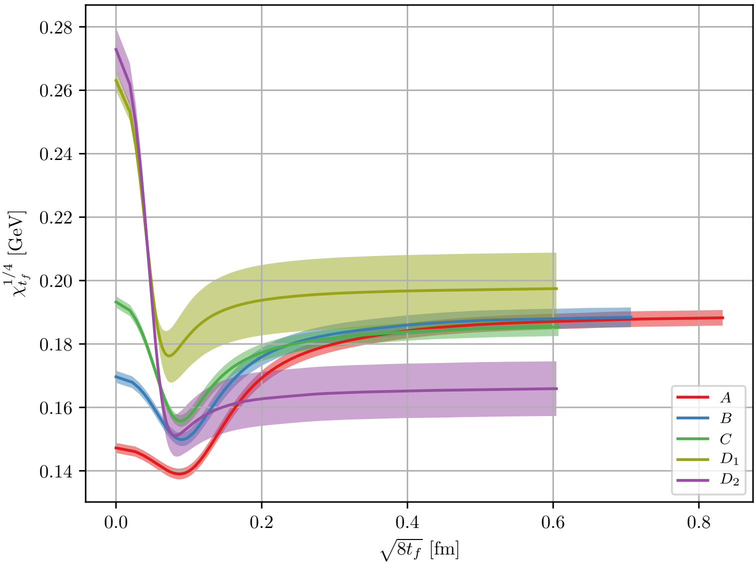


Topological susceptibility continuum extrapolation

Ensembles	$\chi_{t_f}^{1/4}\left(\langle Q^2 \rangle\right)$ [GeV]	N_f	$\chi^2/\mathrm{d.o.f}$
A, B, C, D_2	$0.179(10)$	$3.75(29)$	2.38
A, B, C, D_1	$0.186(6)$	$3.21(25)$	0.83
A, B, C	$0.184(6)$	$3.37(26)$	0.33

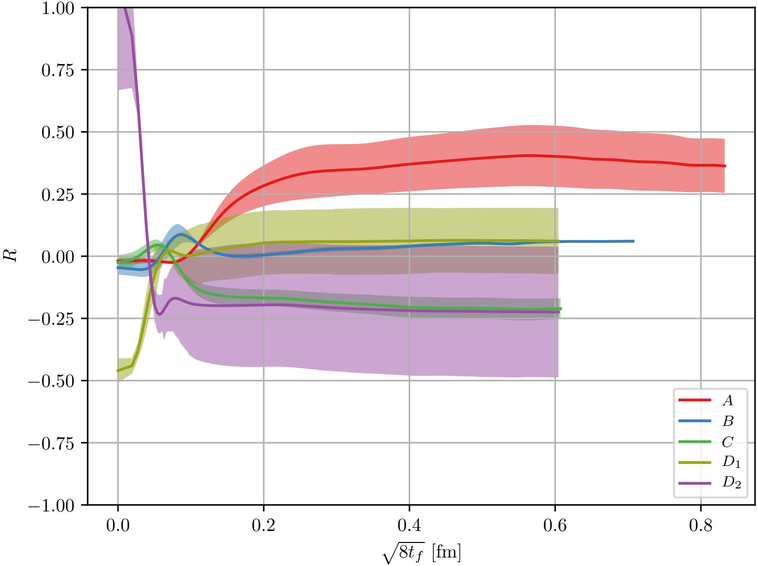
The fourth cumulant

$$\left\langle Q^4 \right\rangle_c = \frac{1}{V^2} \left(\left\langle Q^4 \right\rangle - 3 \left\langle Q^2 \right\rangle^2 \right).$$

From this, we can also measure the ratio R,

$$R = \frac{\left\langle Q^4 \right\rangle_c}{\frac{1}{V} \left\langle Q^2 \right\rangle} = \frac{1}{V} \frac{\left\langle Q^4 \right\rangle - 3 \left\langle Q^2 \right\rangle^2}{\left\langle Q^2 \right\rangle},$$

The fourth cumulant



The fourth cumulant at reference flow times

Ensemble	L/a	t_0/a^2	$\langle Q^2 \rangle$	$\langle Q^4 \rangle$	$\langle Q^4 \rangle_C$	R
A	2.24	3.20(3)	0.78(4)	2.13(27)	0.282(67)	0.359(65)
B	2.21	4.43(4)	0.81(5)	1.98(23)	0.036(11)	0.044(11)
C	2.17	6.01(6)	0.77(4)	1.6(2)	−0.174(40)	−0.226(64)
D_1	1.53	12.2(1)	1.00(20)	3.01(1.07)	0.03(12)	0.03(12)
D_2	2.29	12.2(1)	0.497(100)	0.64(20)	−0.103(95)	−0.21(23)

Comparing fourth cumulant

We can compare with article by Cè et al. [2015]

Comparing fourth cumulant

Ensemble	β	L/a	L [fm]	a [fm]	t_0/a^2	t_0/r_0^2	N_{cfg}
F_1	5.96	16	1.632	0.102	2.7887(2)	0.1113(9)	1 440 000
B_2	6.05	14	1.218	0.087	3.7960(12)	0.1114(9)	144 000
$\tilde{D}_2$		17	1.479		3.7825(8)	0.1110(9)	
B_3	6.13	16	1.232	0.077	4.8855(15)	0.1113(10)	144 000
$\tilde{D}_3$		19	1.463		4.8722(11)	0.1110(10)	
B_4	6.21	18	1.224	0.068	6.2191(20)	0.1115(11)	144 000
$\tilde{D}_4$		21	1.428		6.1957(14)	0.1111(11)	

Comparing fourth cumulant

Article	Thesis	Ratio($\langle Q^2 \rangle$)	Ratio($\langle Q^4 \rangle$)	Ratio($\langle Q^4 \rangle_C$)	Ratio(R)
F_1	A	$1.08(6)$	$1.34(18)$	$19.03(5.81)$	$17.64(4.48)$
B_2	A	$1.02(5)$	$1.15(15)$	$3.60(1.09)$	$3.54(90)$
	B	$1.04(6)$	$1.06(11)$	$0.480(74)$	$0.46(4)$
$\tilde{D}_2$	A	$1.02(5)$	$1.19(15)$	$8.31(1.99)$	$8.15(1.56)$
	B	$1.05(6)$	$1.10(12)$	$1.1(1)$	$1.06(3)$
B_3	B	$1.06(6)$	$1.10(12)$	$0.550(86)$	$0.52(5)$
$\tilde{D}_3$	B	$1.05(6)$	$1.11(12)$	$1.51(23)$	$1.4(1)$
B_4	C	$0.99(5)$	$0.86(8)$	$-2.32(46)$	$-2.35(59)$
$\tilde{D}_4$	C	$0.98(5)$	$0.85(8)$	$-3.95(96)$	$-4.05(1.19)$

The topological charge correlator and the effective glueball mass

The **topological charge correlator**

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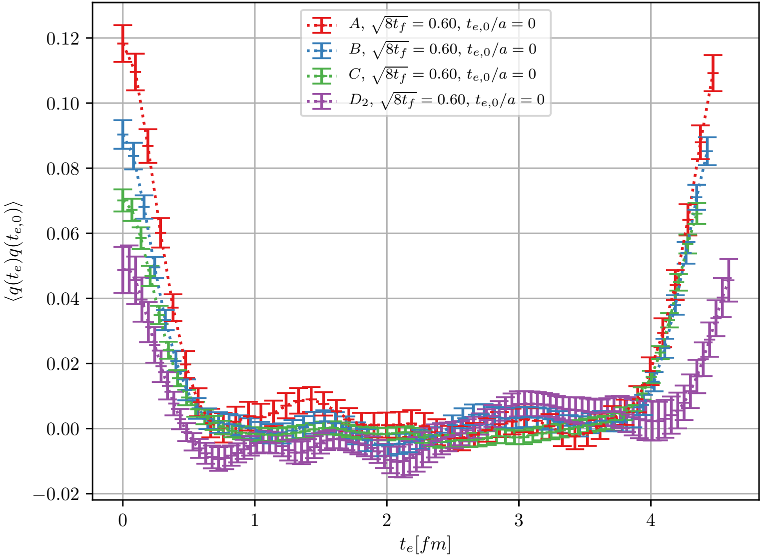
from which the **effective glueball mass** can be extracted as

$$a m_{\mathrm{eff}} = \log\left(\frac{C(n_t)}{C(n_t+1)}\right),$$

The topological charge correlator



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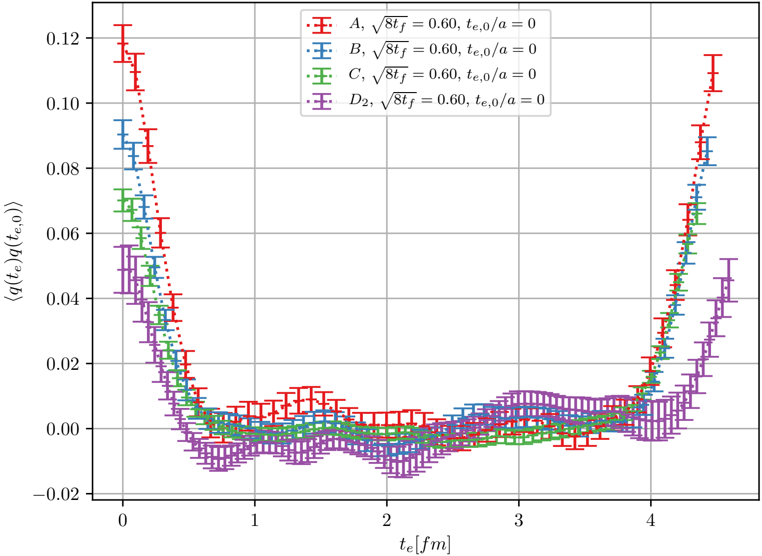

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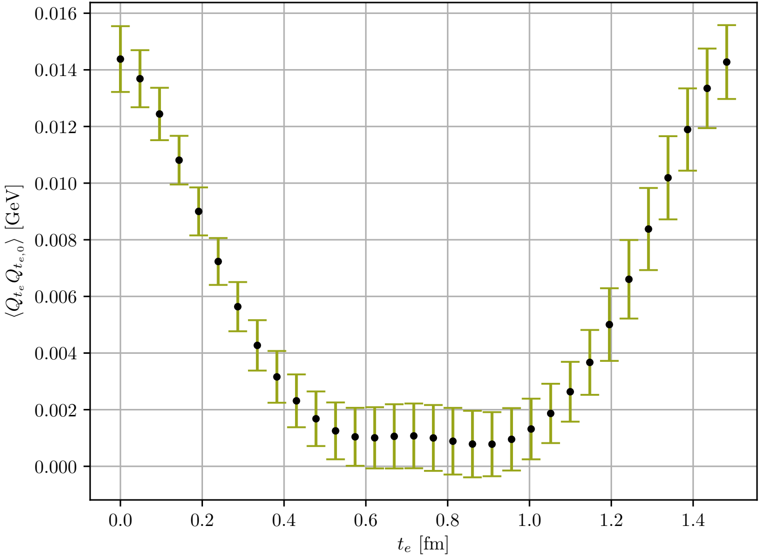
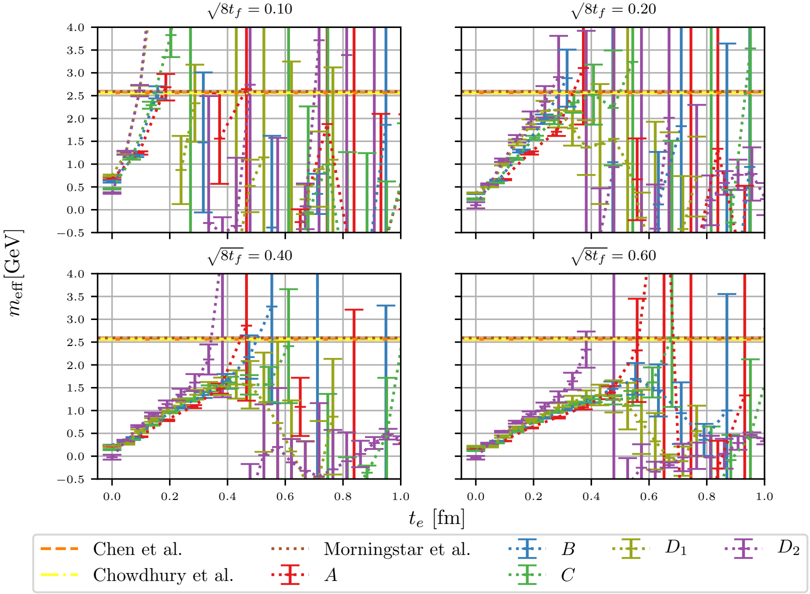


The effective glueball mass



Conclusion, future developments and final thoughts

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- The energy, the scale t_0 and w_0 were also calculated match what is found in the literature, i.e. Lüscher [2010] and Cè et al. [2015].

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- Fermions and HMC(Hybrid Monte Carlo).

Thank you for listening.

Questions?

References

S. Borsanyi, S. Durr, Z. Fodor, C. Hoelbling, S. D. Katz, S. Krieg, T. Kurth, L. Lellouch, T. Lippert, C. McNeile, and K. K. Szabo. High-precision scale setting in lattice QCD. *Journal of High Energy Physics*, 2012(9), September 2012. ISSN 1029-8479. doi: 10.1007/JHEP09(2012)010. URL http://arxiv.org/abs/1203.4469. arXiv: 1203.4469.

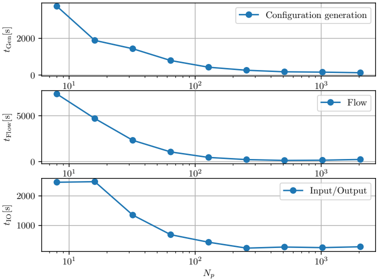
Marco Cè, Cristian Consonni, Georg P. Engel, and Leonardo Giusti. Non-Gaussianities in the topological charge distribution of the SU(3) Yang–Mills theory. *Physical Review D*, 92(7), October 2015. ISSN 1550-7998, 1550-2368. doi: 10.1103/PhysRevD.92.074502. URL http://arxiv.org/abs/1506.06052. arXiv: 1506.06052.

Martin Lüscher. Properties and uses of the Wilson flow in lattice QCD. *Journal of High Energy Physics*, 2010(8), August 2010. ISSN 1029-8479. doi: 10.1007/JHEP08(2010)071. URL http://arxiv.org/abs/1006.4518. arXiv: 1006.4518.

Extra slides

We checked three types of scaling,

- **Strong scaling:** *fixed problem* and a *variable N_p cores*



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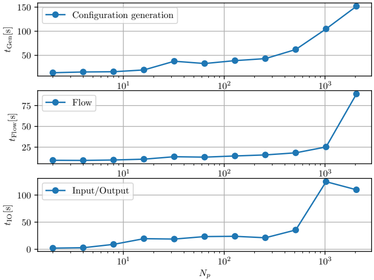

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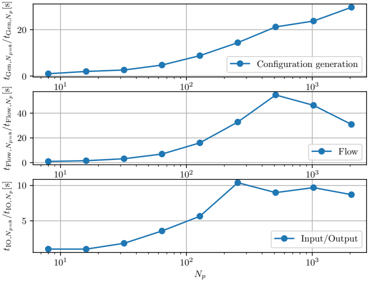

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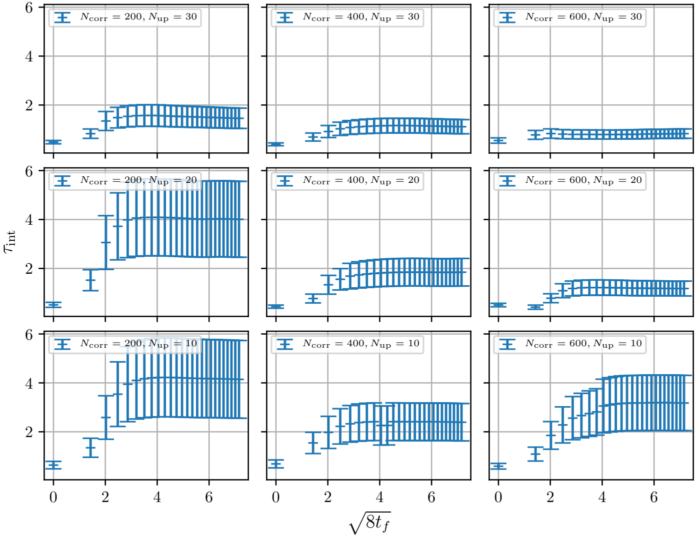
We appear to have a plateau around 512 cores.

Optimizing the gauge configuration generation

Generated 200 configurations for a lattice of size $N^3 \times N_T = 16^3 \times 32$ and $\beta = 6.0$, for combinations of $N_{\text{corr}} \in [200, 400, 600]$ and $N_{\text{up}} \in [10, 20, 30]$.

Optimizing the gauge configuration generation



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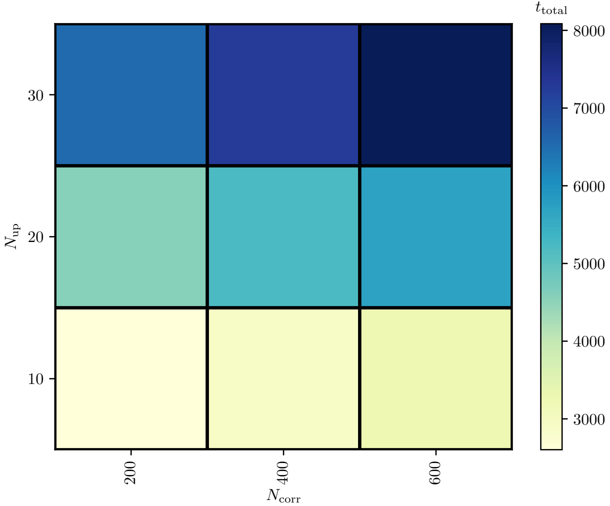

Verifying the code

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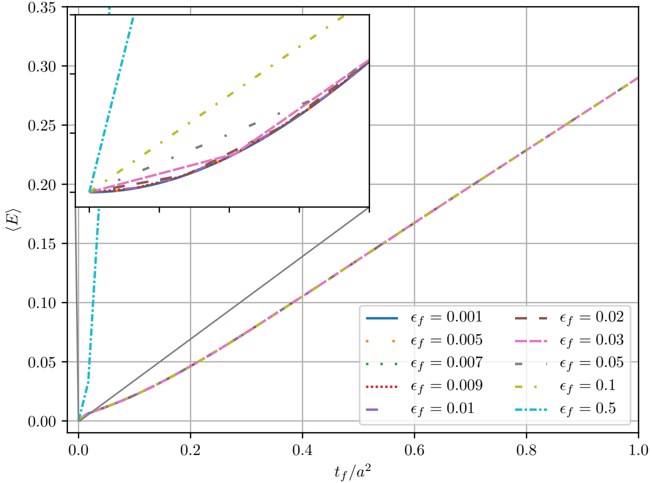
- **Integration testing.** Random matrix generation, lattice objects, parallelization, ect.
- **Validation testing.** Cross checking results with a configuration from Chroma.

Verifying the integration

Testing the integrator for different integration steps ϵ_f.

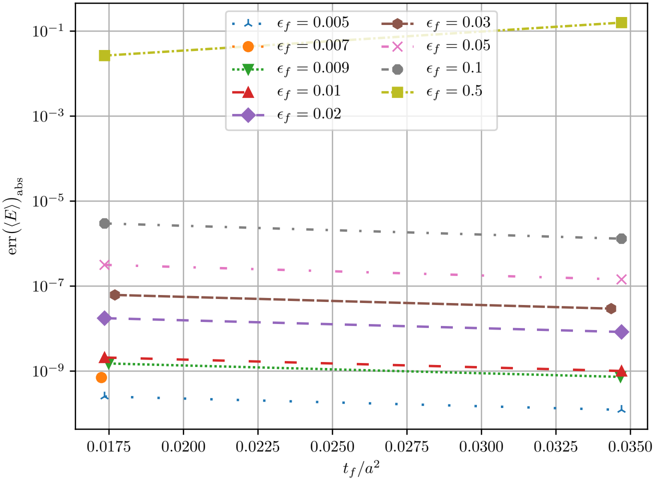
ϵ_f	0.001	0.005	0.007	0.009	0.01	0.02	0.03	0.05	0.1	0.5

Lattice size $N^3 \times N_T = 24^3 \times 48$ with $\beta = 6.0$.



Verifying the integration

The absolute difference between the smallest flow time $\epsilon_f = 0.001$ and those shown previously.



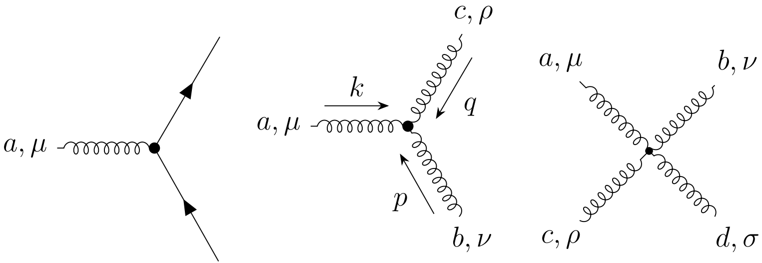
The QCD Lagrangian

$$\mathcal{L}_{\mathrm{QCD}} = \sum_{f=1}^{N_f} \bar{\psi}^{(f)} \left(i\not{D} - m^{(f)} \right) \psi^{(f)} - \frac{1}{4} G^{a}_{\mu\nu} G^{a\mu\nu},$$

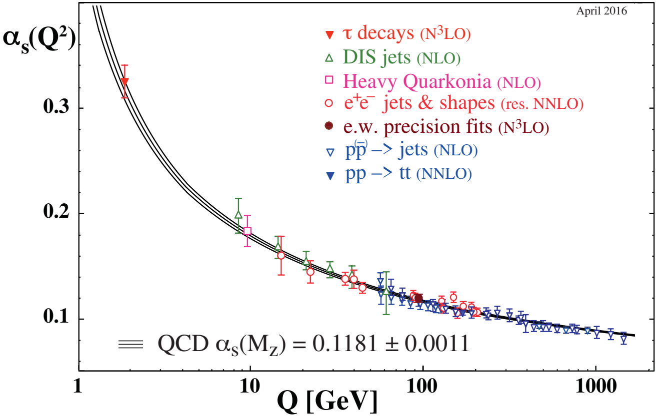
with action

$$S = \int \mathrm{d}^4 x \mathcal{L}_{\mathrm{QCD}}, \tag{1}$$

is invariant under a $\mathrm{SU}(3)$ symmetry.



Asymptotic freedom



Solving gradient flow with Runge-Kutta 3

With

$$\dot{V}_{t_f} = -g_S^2 \left\{ \partial_{x,\mu} S_G[V_{t_f}] \right\} V_{t_f} = Z(V_{t_f}) V_{t_f},$$

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and $Z_i = \epsilon_f Z(W_i)$ we get

$$\begin{aligned}
W_0 &= V_{t_f}, \\
W_1 &= \exp\left[\frac{1}{4} Z_0\right] W_0, \\
W_2 &= \exp\left[\frac{8}{9} Z_1 - \frac{17}{36} Z_0\right] W_1, \\
V_{t_f+\epsilon_f} &= \exp\left[\frac{3}{4} Z_2 - \frac{8}{9} Z_1 + \frac{17}{36} Z_0\right] W_2,
\end{aligned}$$

with coefficients from Lüscher [2010].

Additional ensembles

Ensemble	N	N_T	N_{cfg}	N_{corr}	N_{up}	a [fm]	L [fm]
E	8	16	8135	600	30	0.0931(4)	0.745(3)
F	12	24	1341	200	20	0.0931(4)	1.118(5)
G	16	32	2000	400	20	0.0790(3)	1.265(6)

Energy definition

We use t_0

$$E = \frac{a^4}{2|\Lambda|} \sum_{n \in \Lambda} \sum_{\mu,\nu} \left(F_{\mu\nu}^{\text{clov}}(n) \right)^2$$

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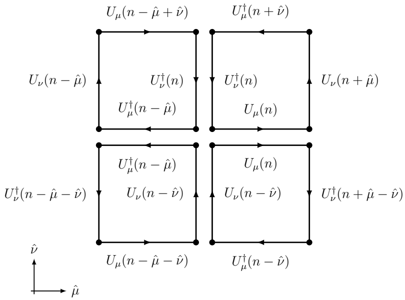
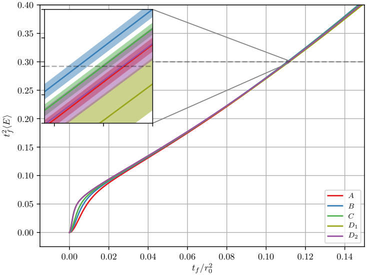
$F_{\mu\nu}^{\text{clov}}(n)$ is given by

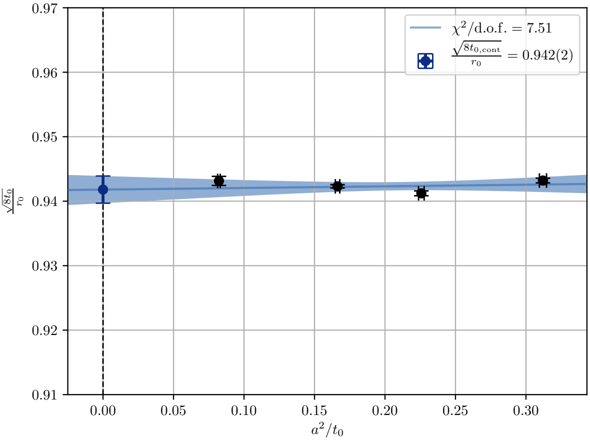


Using scale definition t_0 from Lüscher [2010],

$$\left\{ t_f^2 \left\langle E(t) \right\rangle \right\}_{t_f = t_0} = 0.3.$$

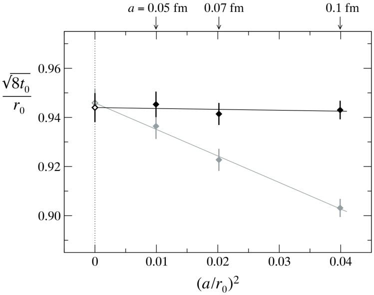


Scale setting t_0



Continuum extrapolation using ensembles A, B, C, and D_2 gives $t_{0,\mathrm{cont}}/r_0^2 = 0.11087(50)$.

This matches the values retrieved by Lüscher [2010],



Scale setting t_0

Ensemble	L/a	L [fm]	a [fm]
A	24	2.235(9)	0.0931(4)
B	28	2.214(10)	0.0791(3)
C	32	2.17(1)	0.0679(3)
D_1	32	1.530(9)	0.0478(3)
D_2	48	2.29(1)	0.0478(3)

Scale setting t_0

Ensemble	$t_0[\text{fm}^2]$	t_0/a^2	t_0/r_0^2
A	$0.02780(2)$	$3.20(3)$	$0.11121(9)$
B	$0.02769(2)$	$4.43(4)$	$0.11075(10)$
C	$0.02775(2)$	$6.01(6)$	$0.11099(8)$
D_1	$0.02779(5)$	$12.2(1)$	$0.1112(2)$
D_2	$0.02794(9)$	$12.2(1)$	$0.1117(3)$

Scale setting t_0

Extrapolations for different ensemble-combinations

Ensembles	$t_{0,\mathrm{cont}}/r_0^2$	$\chi^2/\mathrm{d.o.f}$
A, B, C, D_2	$0.11087(50)$	7.51
B, C, D_2	$0.1115(3)$	0.41
A, B, C, D_1	$0.1119(6)$	0.88

Scale setting w_0

Can also set a scale using the derivative which offers more granularity for small flow times,

$$W(t)|_{t=w_0^2} = 0.3,$$
$$W(t) \equiv t_f \frac{\mathrm{d}}{\mathrm{d}t_f} \left\{ t_f^2 \langle E \rangle \right\}.$$

First presented by Borsanyi et al. [2012].

Scale setting w_0

Ensembles	$w_{0,\mathrm{cont}}$[fm]	$\chi^2/\mathrm{d.o.f}$
A, B, C, D_2	$0.1695(5)$	7.12
B, C, D_2	$0.1702(3)$	0.53
A, B, C, D_1	$0.1706(6)$	0.86

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A, B, C, D_2	$0.1695(5)$	7.12
B, C, D_2	$0.1702(3)$	0.53
A, B, C, D_1	$0.1706(6)$	0.86

Comparable to Borsanyi et al. [2012] which included dynamical fermions, with $w_{0,\mathrm{cont}} = 0.1755(18)(04)$ fm.

Autocorrelation in the energy