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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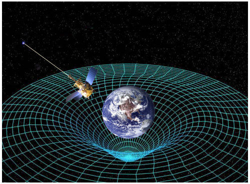
Co-supervisor: *Morten Hjorth-Jensen*

University of Oslo

The four forces of nature



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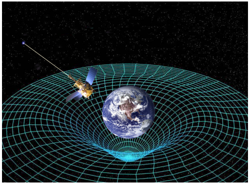

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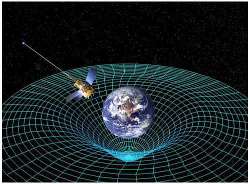

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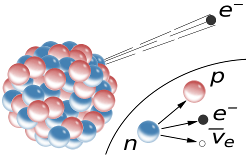

Weak nuclear force

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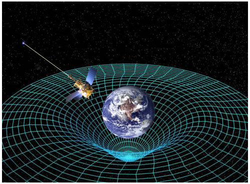

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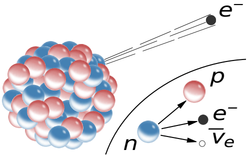

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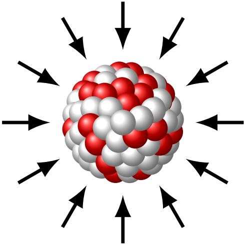

Strong nuclear force

What is the strong force?

Consists of:

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

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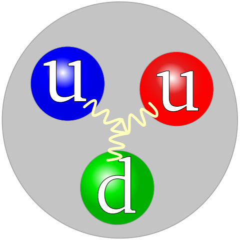

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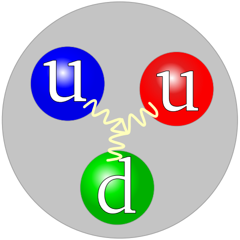
Mass discrepancy:

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

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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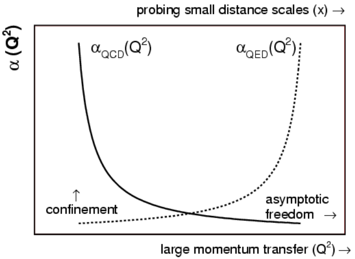

https://www-cdf.fnal.gov/~group/WORK/DISS_PAGE/diss_page.htm

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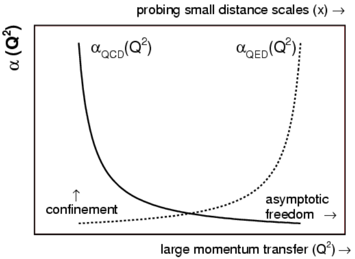

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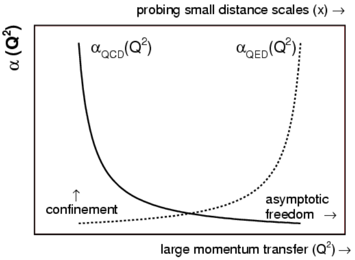

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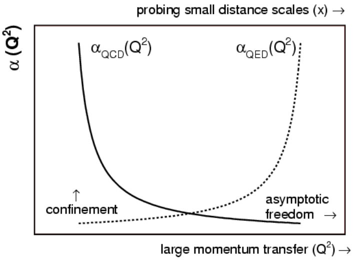

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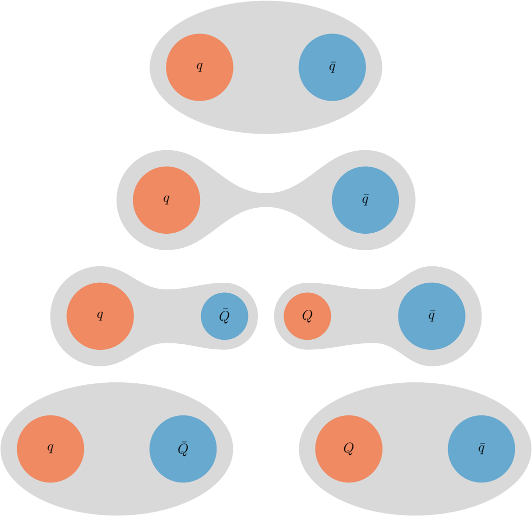
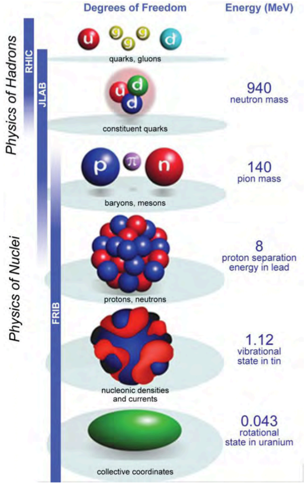
- Coupling constant α is the strength of the force in an interaction.
- QED becomes stronger - QCD becomes weaker at higher energies.
- Can't use perturbation theory on strong force in low-energy regime!
- Need to understand the low-energy regime to understand phenomenas such as **confinement**.

Confinement: a low-energy phenomena

No free quarks in nature!



QCD and nuclear physics



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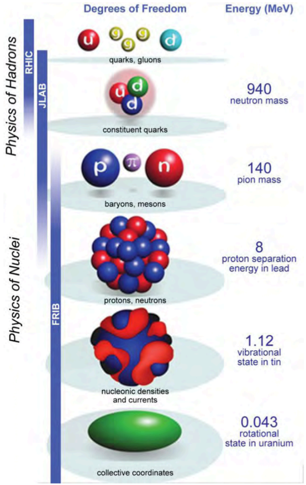

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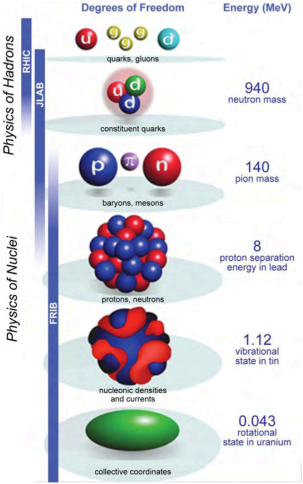

- Need to understand the low-energy regime in order to better understand nuclear physics!
- Want to bridge the gap between theories that operate at different scales.
- $\rightarrow$ numerical methods(e.g. lattice QCD)

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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

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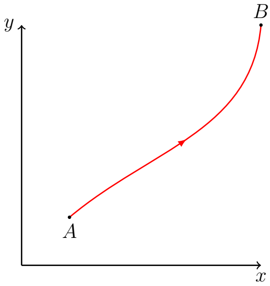

Classically, only one possible path obtained from the principle of least action.

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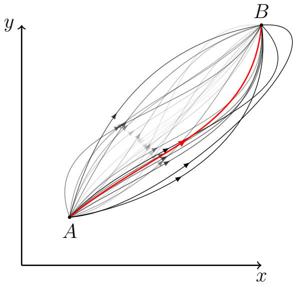

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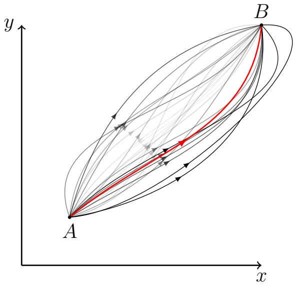

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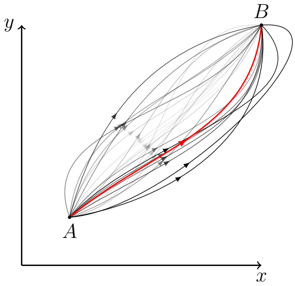

In quantum mechanics, there is lots of possible paths.
Principle of least action (or stationary condition): $\frac{\delta}{\delta x(t)}\left(S\left[x(t)\right]\right) = 0$
Sum over all possible paths $\rightarrow$ the most likely path.

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})! \\
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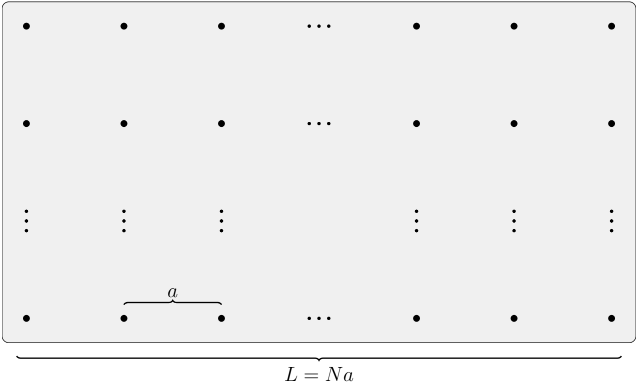
Difficult to calculate the all possible paths $\to$ discretize spacetime

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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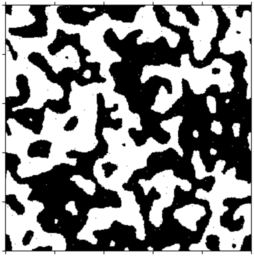
- With $N = 10$, a lattice in the Ising model has the size $10 \times 10 = 100$.
- A lattice in LQCD is however $N^4 = 10000$.

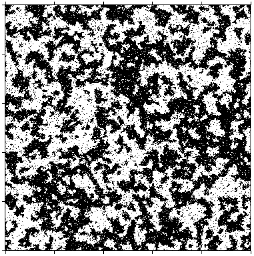
Then what is a configuration?

Looking at a spin lattice of the Ising model,

$T = 1.10$



$T = 2.10$



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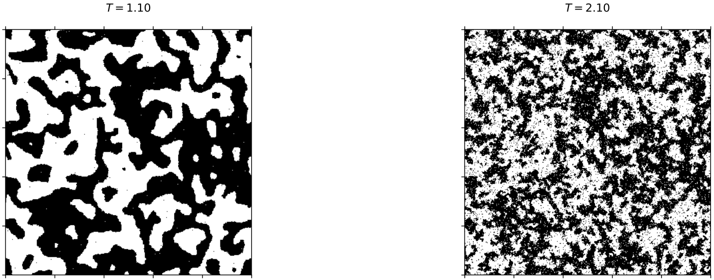

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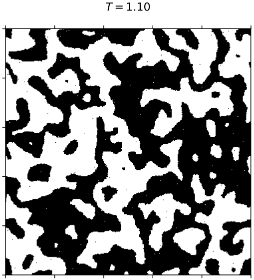

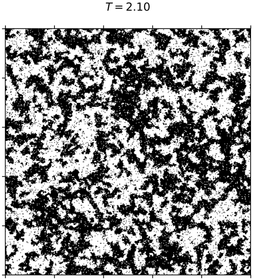

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- A **configuration** in LQCD is a given *arrangement of the gauge field*.

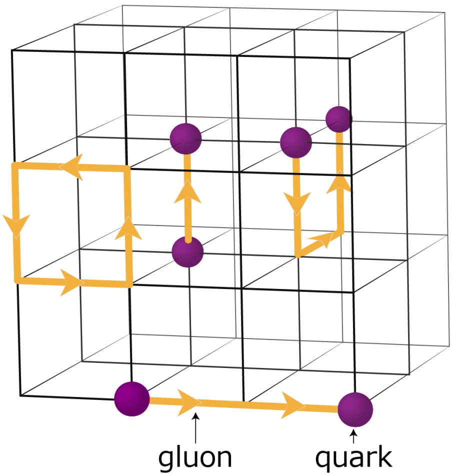
Sampling configurations

An expectation value becomes

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

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 $\beta = 6/g_S^2$

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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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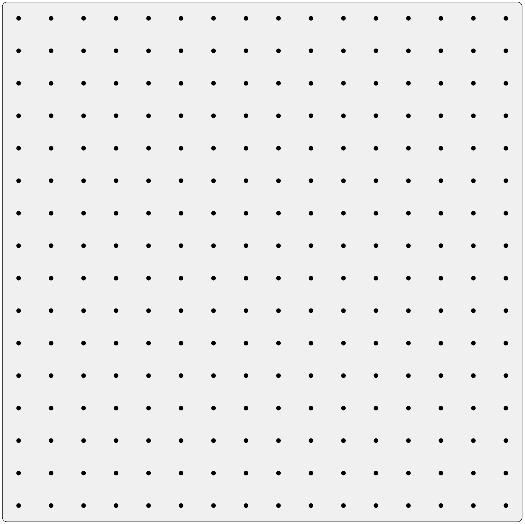
Too large to solve on any single computer.

Parallelization: splitting the hypercube



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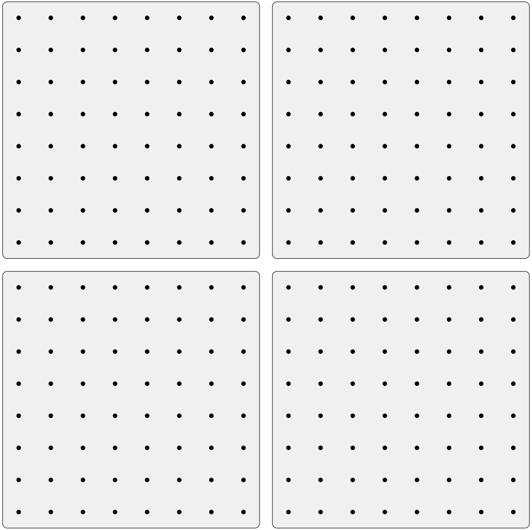

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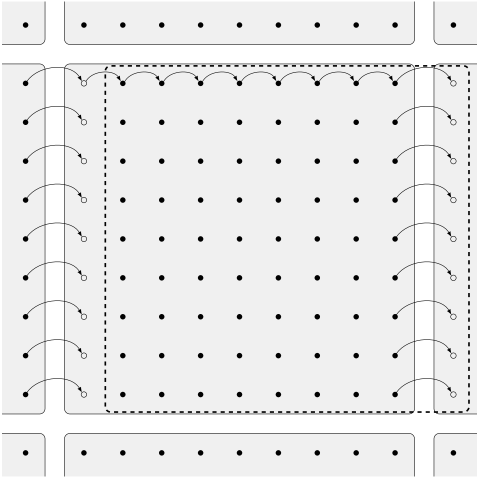

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However, some observable are problematic...

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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[1] Lüscher [2010]

Gradient flow

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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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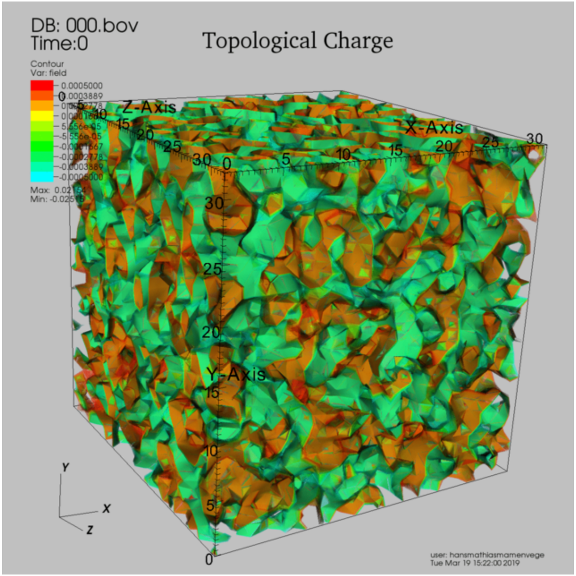
Gradient flow III: topological charge



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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$$Q = a^4 \sum_{n \in \Lambda} q(n),$$

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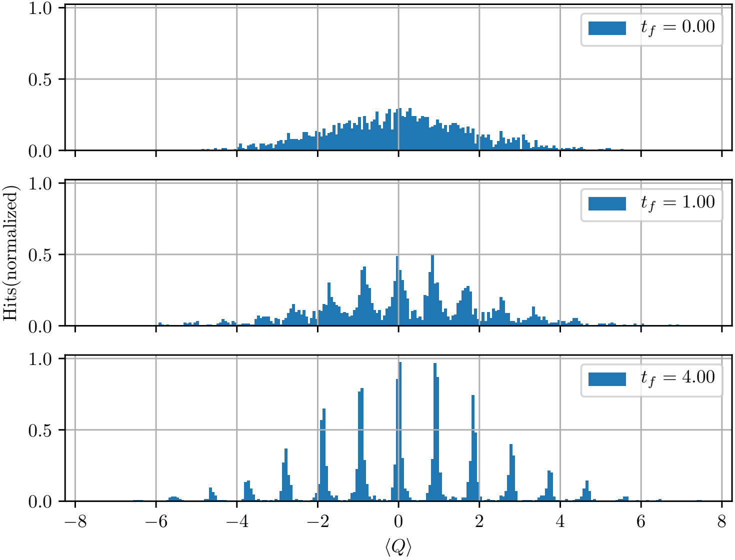
Integer valued and equally probably to have negative charge as positive,

$$\langle Q \rangle = 0$$

Topological charge distribution



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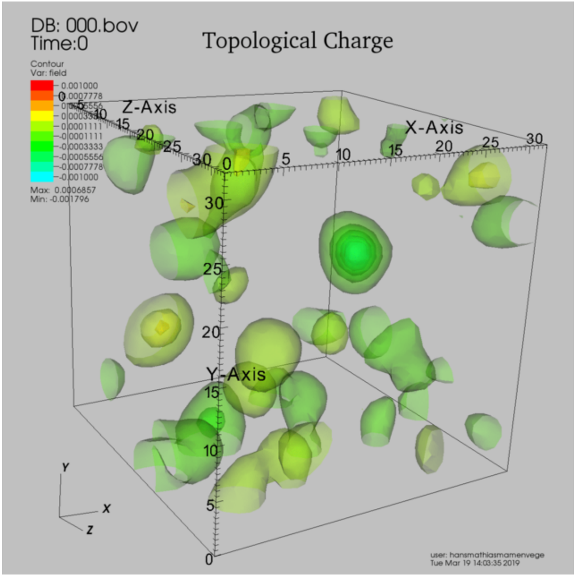
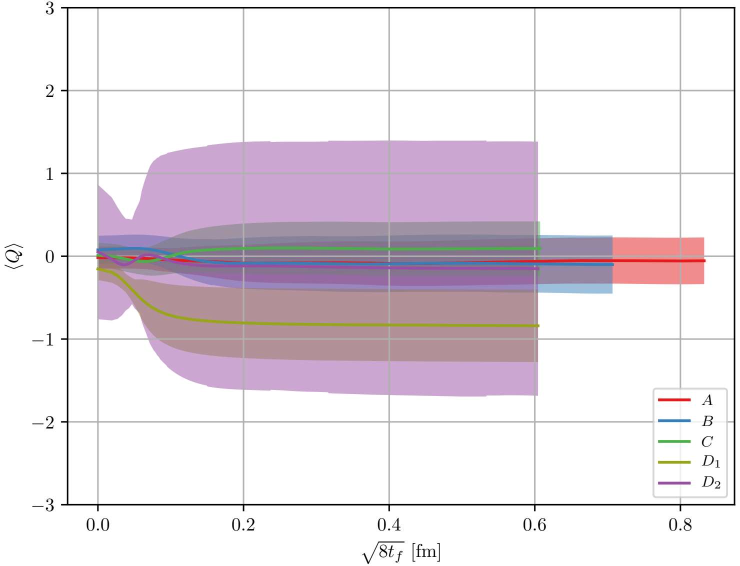


Topological charge for our main ensembles



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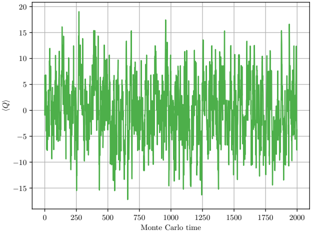
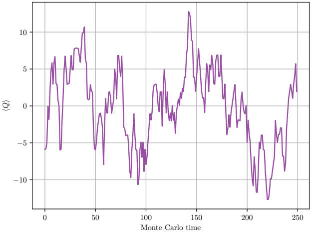
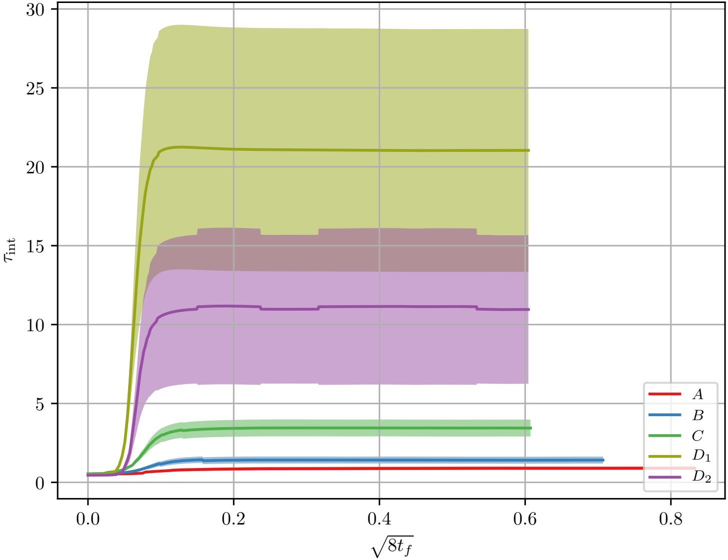


Ensemble C, $32^3 \times 64$, $\beta = 6.2$



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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The *topological susceptibility* is given by

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

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We expect $N_f = 3$.

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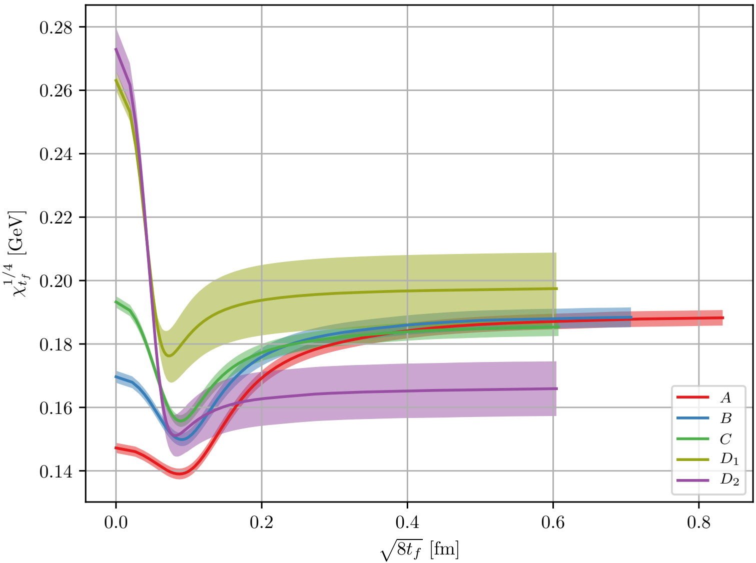

Topological susceptibility continuum extrapolation

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,

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

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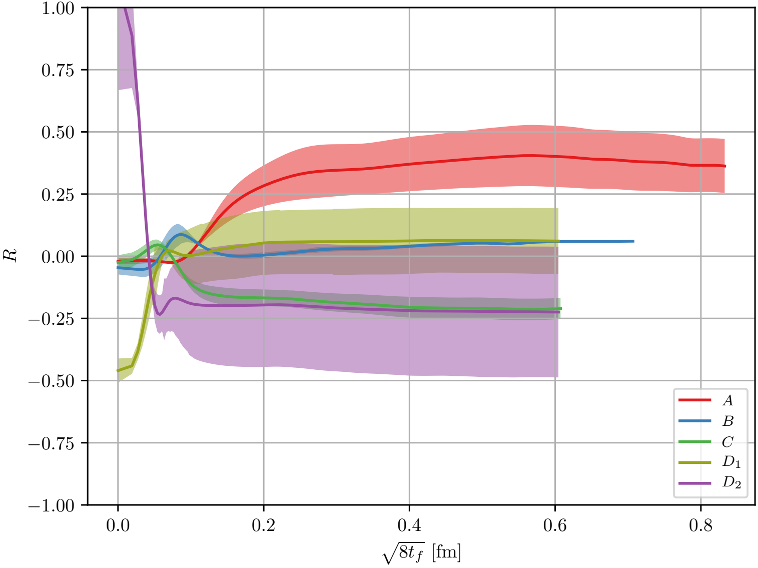

The fourth cumulant at reference flow times

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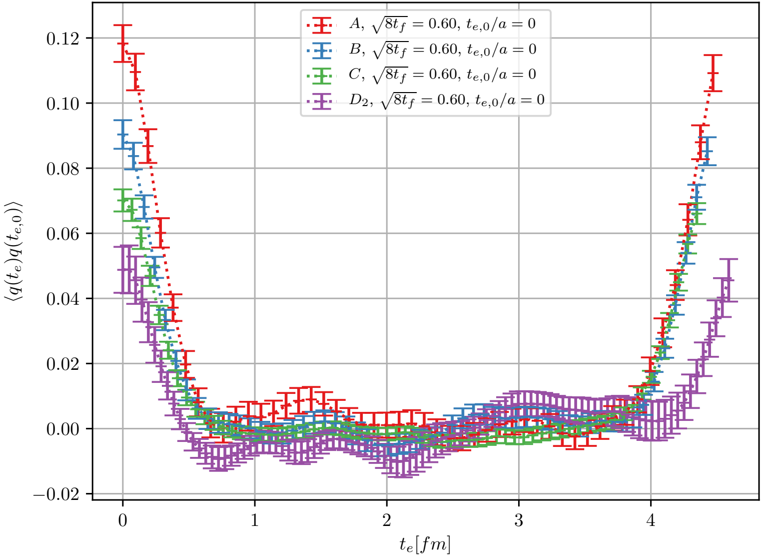
from which the **effective glueball mass** can be extracted as

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

The topological charge correlator



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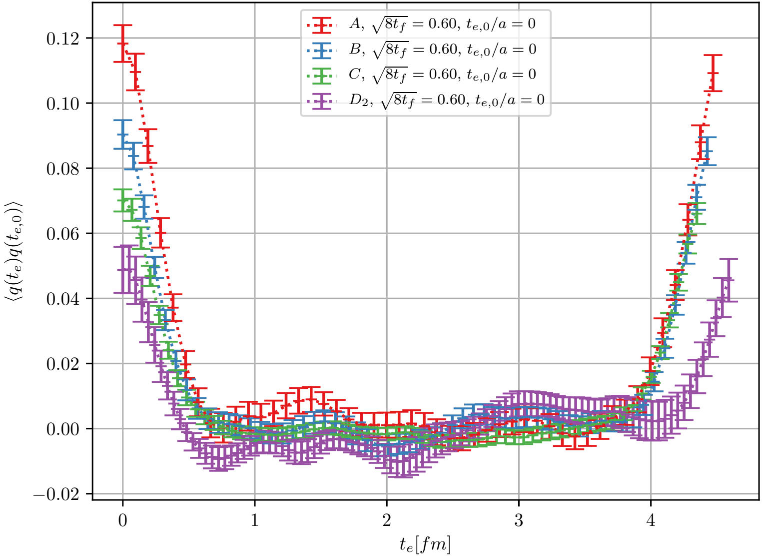

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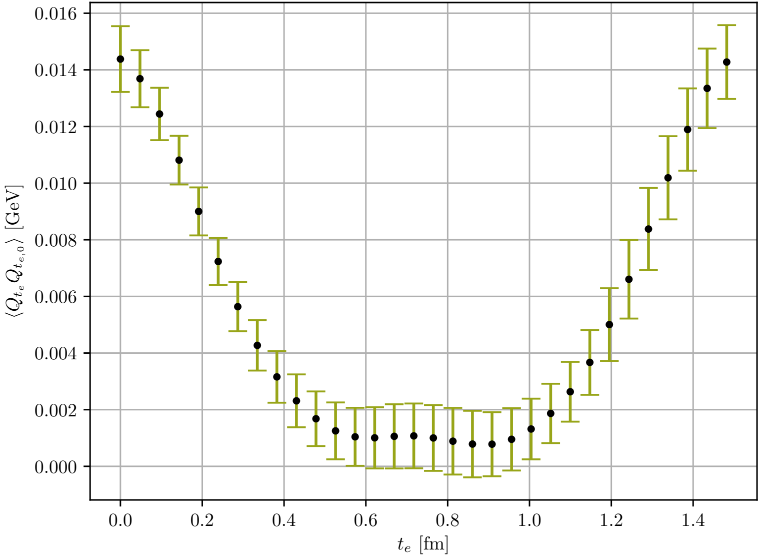
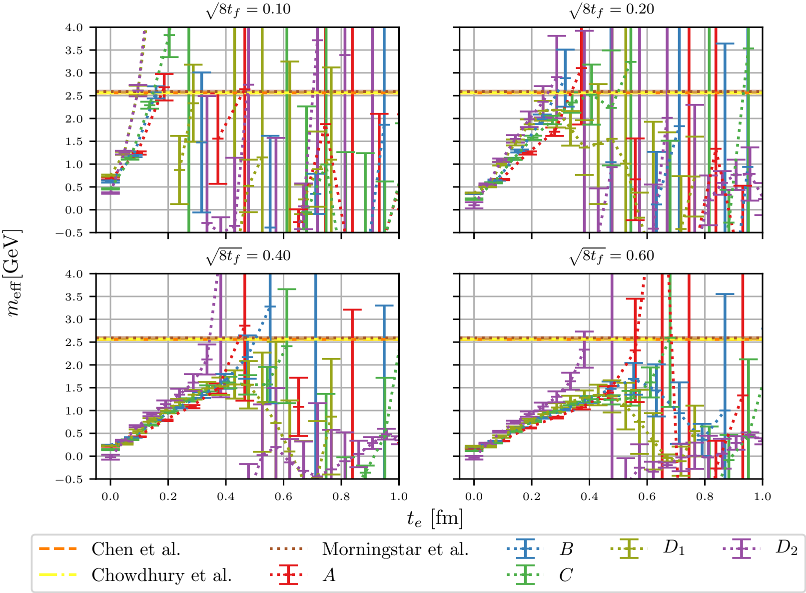


The effective glueball mass



Conclusion, future developments and final thoughts

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- Fermions and HMC(Hybrid Monte Carlo).

Thank you for listening.

Questions?

References

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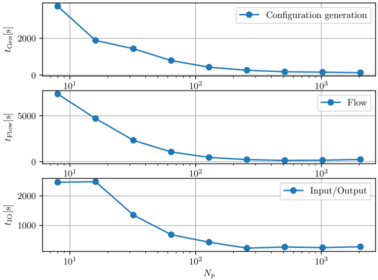
Extra slides

Scaling

We checked three types of scaling,

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



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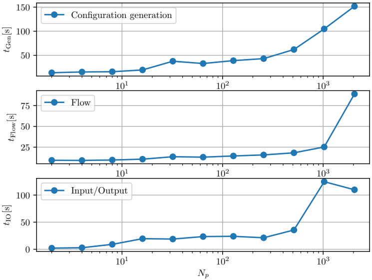
- **Weak scaling:** *fixed problem per processor* and a *variable N_p cores*.



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We checked three types of scaling,

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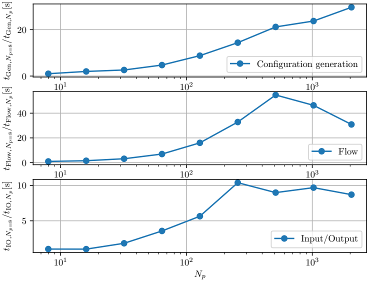

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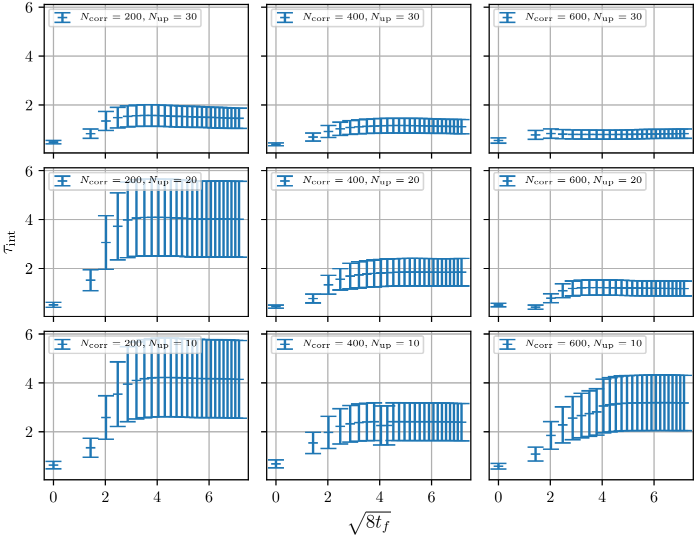
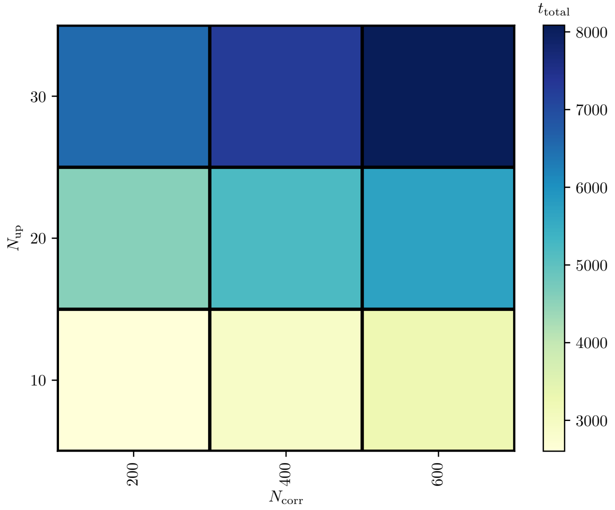
We appear to have a plateau around 512 cores.

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 $N_{\mathrm{corr}} \in [200, 400, 600]$ and $N_{\mathrm{up}} \in [10, 20, 30]$.

Optimizing the gauge configuration generation




t_{total}
8000
7000
6000
5000
4000
3000
30
20
10
N_{up}
200
400
600
N_{corr}

Verifying the code

- Unit testing. $\mathrm{SU}(3)$, $\mathrm{SU}(2)$ multiplications.

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

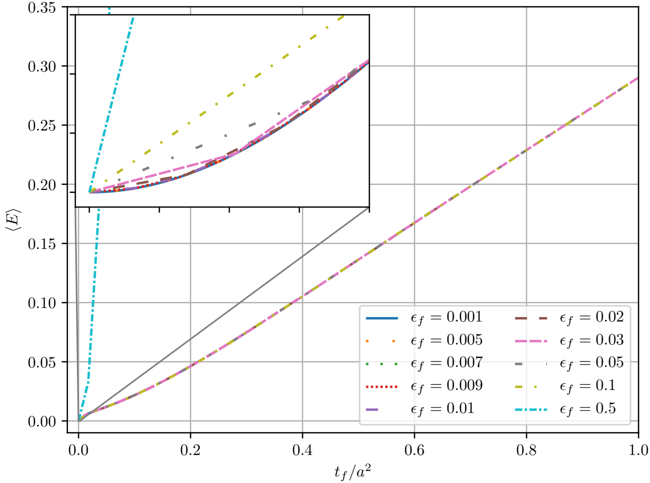
Verifying the integration

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

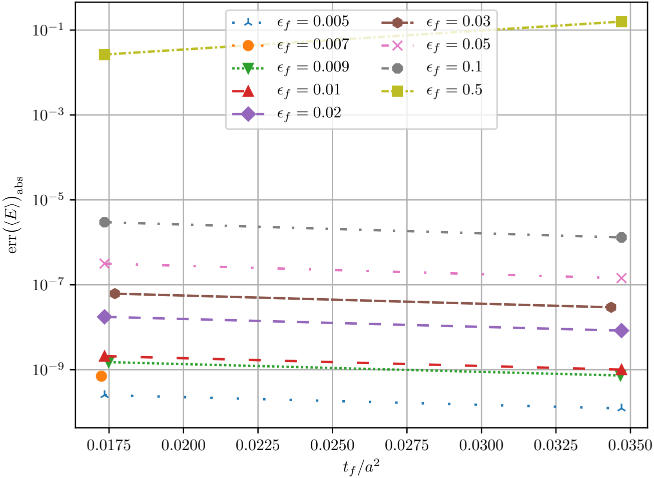
Verifying the integration

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.



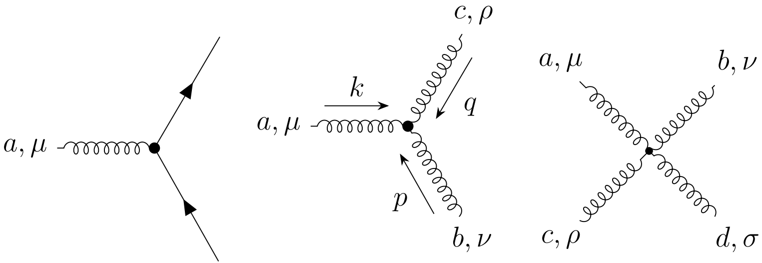
The QCD Lagrangian

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

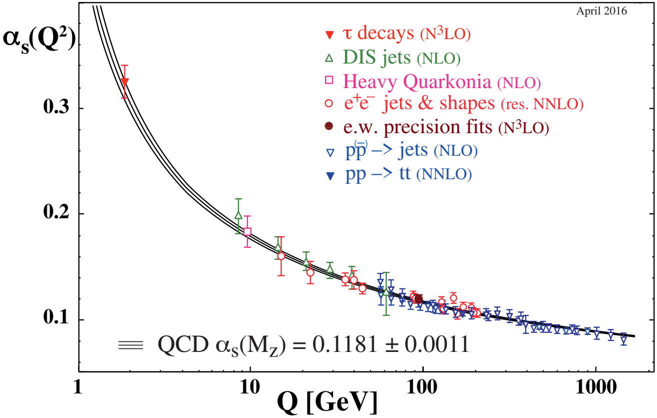
with action

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

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

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

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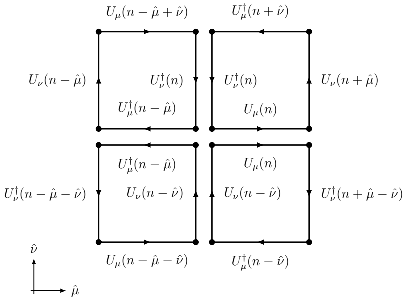
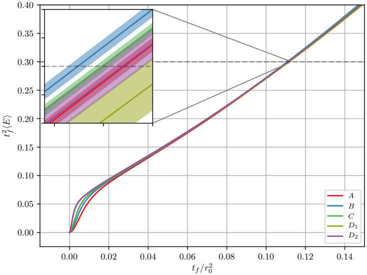
$F^{\text{clov}}_{\mu\nu}(n)$ is given by

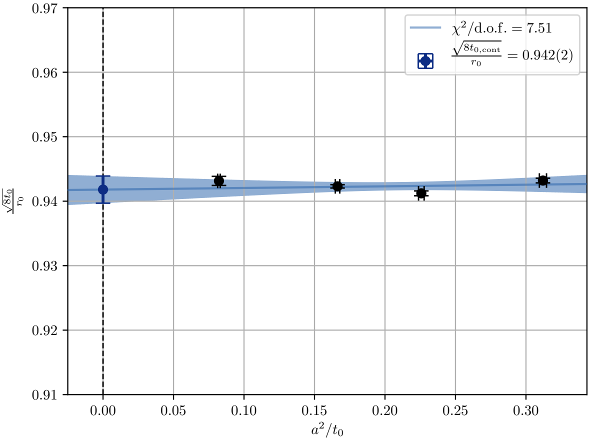


Using scale definition t_0 from Lüscher [2010],

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



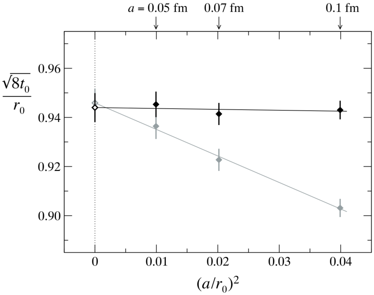
Scale setting t_0



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

Scale setting t_0

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	$t_0[\mathrm{fm}^2]$	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

Scale setting w_0

Ensembles	$w_{0,\mathrm{cont}}$[fm]	χ^2/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

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

Autocorrelation in the energy