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

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University of Oslo

Introduction

Structure

- Quantum Chromodynamics(QCD).

1

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- **Results.** We will present the results obtained from pure gauge calculations.

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Quantum Chromodynamics(QCD)

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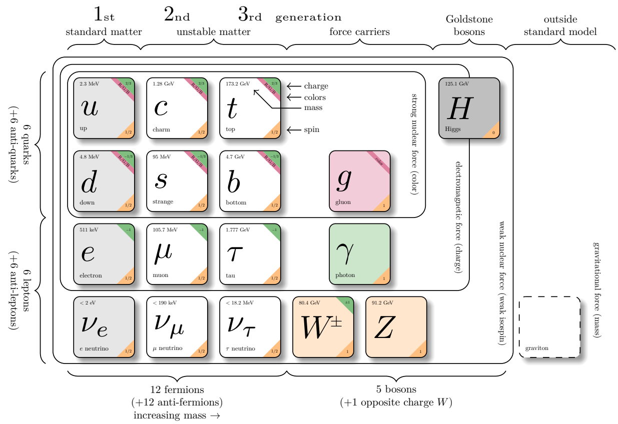
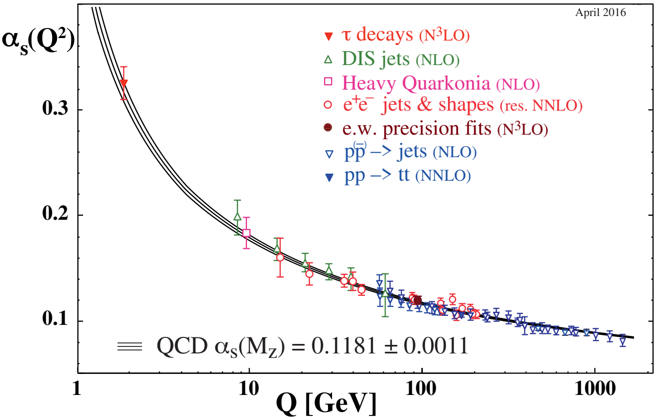
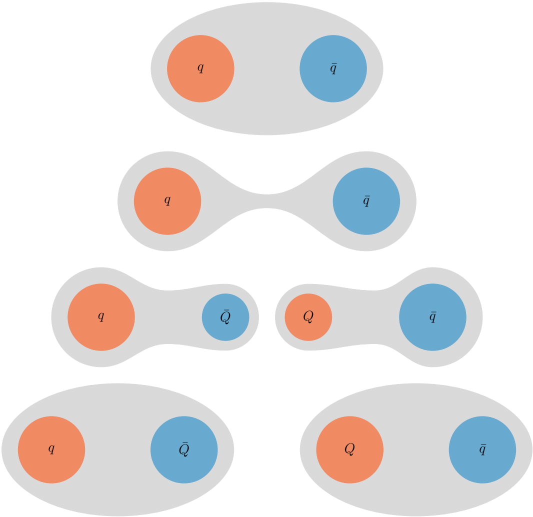
The Standard Model



Consists of the innermost square of the six quarks and the gluons.



- The coupling constant **decreases** as we **increase** the energy
- One of the experimental proofs of QCD along with triple γ decay and muon cross section ration R.



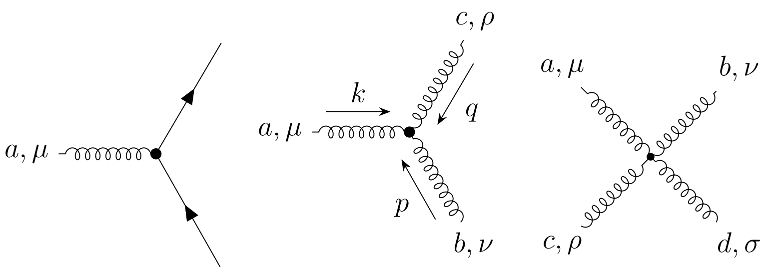
If we try to pull apart **two mesons**, more and more energy is required until we have enough energy to spontaneously create a **quark-antiquark** pair, forming thus **two new mesons.**

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

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



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- **Instantons** are local minimums to the Yang-Mills action in Euclidean space.

Topology in QCD

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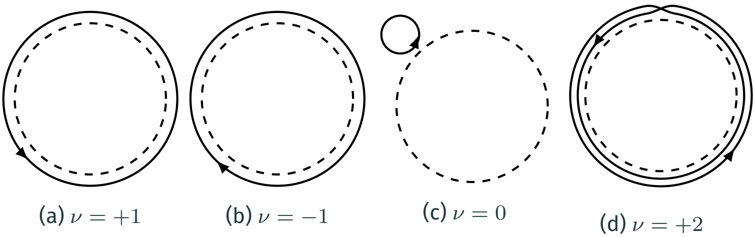

Figure 1: The figure is taken from Forkel [1, p. 32].

- **Instantons** are local minimums to the Yang-Mills action in Euclidean space.
- Measuring **topological charge** is a measure of the *Winding number* of the gauge field.
- An illustration of how one can view the winding number given a function f that parametrizes a path around a circle S^1. Given that it starts and ends at the same point, we have that the number of times it wraps around the circle gives us the winding number.

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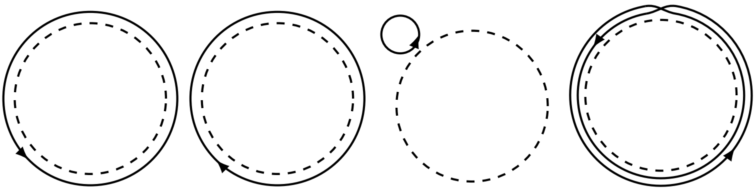

(a) $\nu = +1$ (b) $\nu = -1$ (c) $\nu = 0$ (d) $\nu = +2$

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The Witten-Veneziano relation

A formula connecting pure gauge theory and full QCD.

$$m_{\eta'}^2 = \frac{2N_f}{f_\pi^2}\chi_{\mathrm{top}} \qquad (2)$$

- Pion decay constant $f_\pi = 0.130(5)/\sqrt{2}$ GeV.
- η' meson mass $m_{\eta'} = 0.95778(6)$ GeV.
- χ_{top} is the *topological susceptibility*.

- We use the experimental values for the pion decay constant and the η' mass.
- Allows us to estimate the number of flavors in our theory N_f.
- χ_{top} is the topological susceptibility, calculated from the expectation value of Q.

Lattice Quantum Chromodynamics(LQCD)

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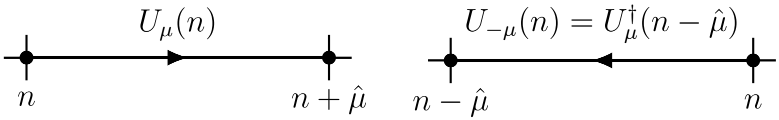
2. Fermions live on the each *point* in the cube.
3. The gauge fields live on the sites *in between* the points, and is called links.

Links

A link

$$U_\mu(n) = \exp\left[iaA_\mu(n)\right],$$

connects one lattice site to another and is a $\mathrm{SU}(3)$ matrix.



where $U_{-\mu}(n) = U_\mu(n-\hat{\mu})^\dagger$.

- Defined from the gauge transporter.
- A link in the positive $\hat{\mu}$ direction is shown in the figure to the left.
- A link in the negative $\hat{\mu}$ direction is shown in the figure to the right.

Gauge invariance on the lattice

Links gauge transform as

$$\begin{aligned} U_\mu(n) &\to U'_\mu(n) = \Omega(n)\, U_\mu(n) \Omega(n+\hat{\mu})^\dagger, \\ U_{-\mu}(n) &\to U'_{-\mu}(n) = \Omega(n)\, U_\mu(n-\hat{\mu})^\dagger \Omega(n-\hat{\mu})^\dagger. \end{aligned}$$

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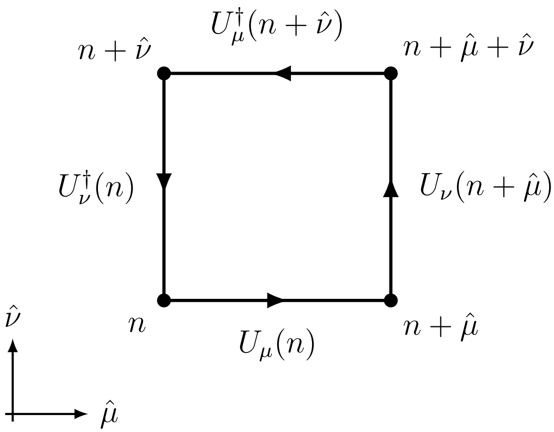
Two main types of gauge invariant objects,

- Fully connected gauge invariant objects.
- Objects with fermions ψ, $\bar{\psi}$ as end points.

The plaquette

The simplest gauge invariant object,

$$\begin{aligned} P_{\mu\nu}(n) &= U_\mu(n)\,U_\nu(n+\hat{\mu})\,U_{-\mu}(n+\hat{\mu}+\hat{\nu})\,U_{-\nu}(n+\hat{\nu}) \\ &= U_\mu(n)\,U_\nu(n+\hat{\mu})\,U_\mu(n+\hat{\nu})^\dagger\,U_\nu(n)^\dagger, \end{aligned}$$



The Wilson gauge action

The Wilson gauge action is given as

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

with $\beta = 6/g_S^2$.

- Using the definition of the link we saw earlier, we can reproduce the continuum action up to an discretization error of $\mathcal{O}(a^2)$.

Developing a code for solving $\mathrm{SU}(3)$ Yang-Mills theory on the lattice

A lattice configuration consists of $\mathrm{SU}(3)$ matrices,

- The $\mathrm{SU}(3)$ matrices are 3×3 matrices of nine complex numbers or 18 real numbers.
- This leads to an absolute **requirement of efficiency**, both in **calculations** and in **input/output**.
- When returning to what ensembles of configurations we generated this will be evident.

The numerical challenge in lattice QCD

A lattice configuration consists of $\mathrm{SU}(3)$ matrices,

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

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$\rightarrow 8 \times 72N^3N_T$ bytes.

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The path integral I

$$\langle O\rangle = \frac{1}{Z}\int \mathcal{D}U O[\psi,\bar{\psi},U]\mathrm{e}^{-S_G[U]-S_F[\psi,\bar{\psi},U]}.$$

with

$$Z = \int \mathcal{D}U\mathcal{D}\bar{\psi}\mathcal{D}\psi\, e^{-S_G[U]-S_F[\psi,\bar{\psi},U]}.$$

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

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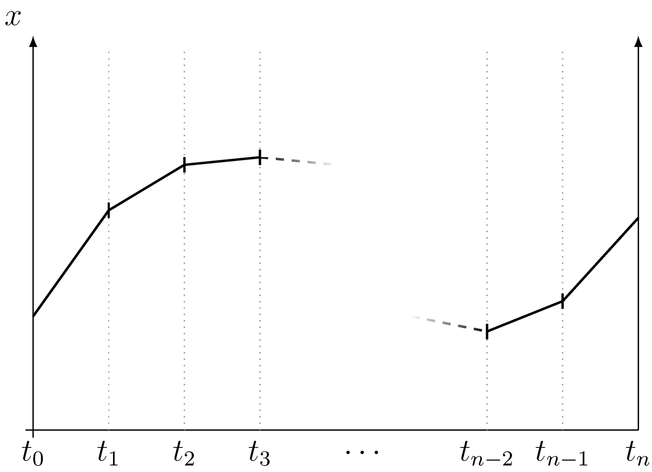


An example of the discretized path integral, going from time t_0 to t_{N_T}, where the end points is taken to be equal, $x_0 = x_{N_T}$. We integrate over all of space at each time t_i finding the most likely position at a given time.

How to measure

The observable becomes an average over the N_{MC} gauge configurations.

$$\langle O \rangle = \lim_{N_{\mathrm{MC}} \to \infty} \frac{1}{N_{\mathrm{MC}}} \sum_{i}^{N_{\mathrm{MC}}} O[U_i]$$

We now need to generate configurations...

- We perform an average of the created configurations.

repeat
Randomly generate a candidate state j with probability $T_{i \to i}$.
Calculate $A_{i \to j}$ which saw on previous slide.
Generate random number $u \in [0, 1]$.
if $u \leq A_{i \to j}$ **then**
Accept new state j.
else if $u > A_{i \to j}$ **then**
Reject new state j and retain the old state i.
end if
until N_{MC} samples are generated.

- Generated state j is a gauge configuration.
- Algorithm of choice when sampling gauge configurations.
- For generating N_{MC} Monte Carlo samples.

The Metropolis algorithm on the lattice

A parameter ϵ_{rnd} controls the spread of the candidate matrices.

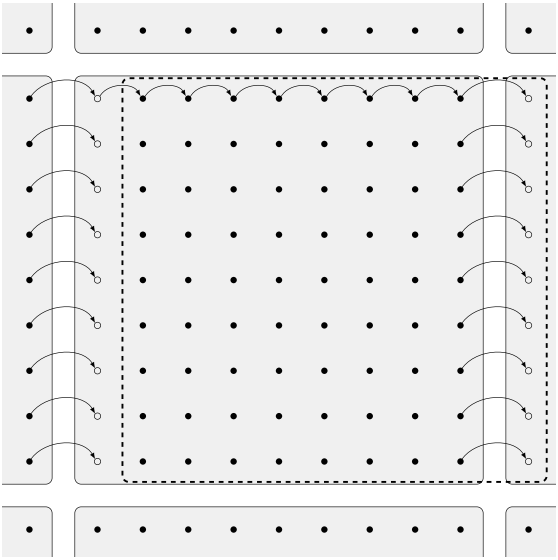
1. Initialize lattice with $\mathrm{SU}(3)$ matrices close to unity(*hot start*) or at unity(*cold start*).
2. Thermalize with N_{therm} sweeps.
3. Generate N_{MC} samples,
   i Perform N_{corr} correlation updates.
   ii At each update, perform N_{up} single link update for every lattice link.
   iii Store configuration and/or apply gradient flow and sample observables on it.

- We use **periodic boundary conditions** for all calculations.
- N_{MC} is how many configurations we will generate.
- N_{up} is how many single link updates we will perform.
- N_{corr} is how many full sweeps we shall perform in between each sampling. Needed in order to reduce the autocorrelation between the configurations.

Two methods used:

- Single link sharing used in the Metropolis algorithm.
- *shifts* used in in gradient flow and observable sampling

- Tested out halos, but turned out to be problematic when generating.
- We parallelized using MPI.

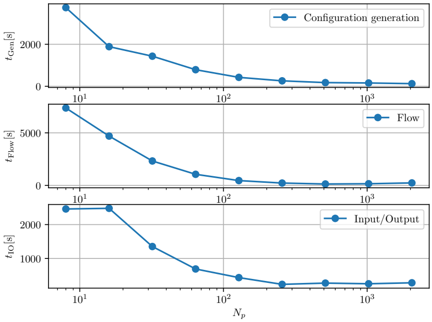


- An illustration of the lattice shift.
- The links U_ν of the lattice are copied over to a temporary lattice shifted in direction $\hat{\mu}$.
- The face that is shifted over to an adjacent sub-lattice is shared through a non-blocking MPI call, while we copy the links to the temporary lattice.
- Allows for a simplified syntax close to that of the equations we are working with.
- Don't have to write out any loops over the lattice positions.

Scaling

We checked three types of scaling,

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



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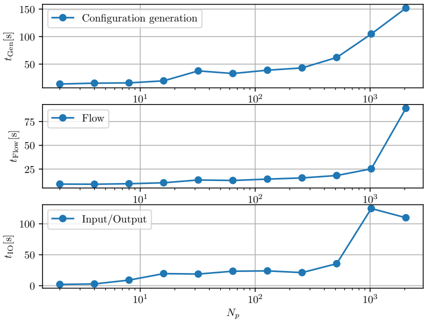

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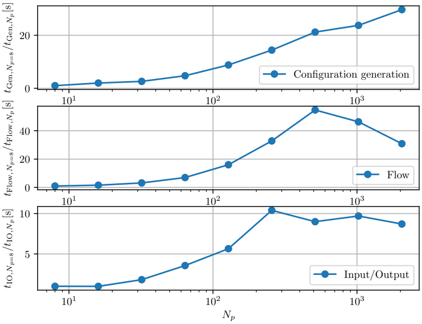
- **Weak scaling:** *fixed problem per processor* and a *variable N_p cores.*
- **Speedup:** defined as $S(p) = \frac{t_{N_p,0}}{t_{N_p}}$.



- Strong scaling
- Weak scaling
- The speedup of the configuration generation, flowing, and IO. The speedup is calculated by dividing the run time of each N_p run, with the run time of the run with the least number of processors, $N_p = 8$.

We appear to have a plateau around 512 cores.

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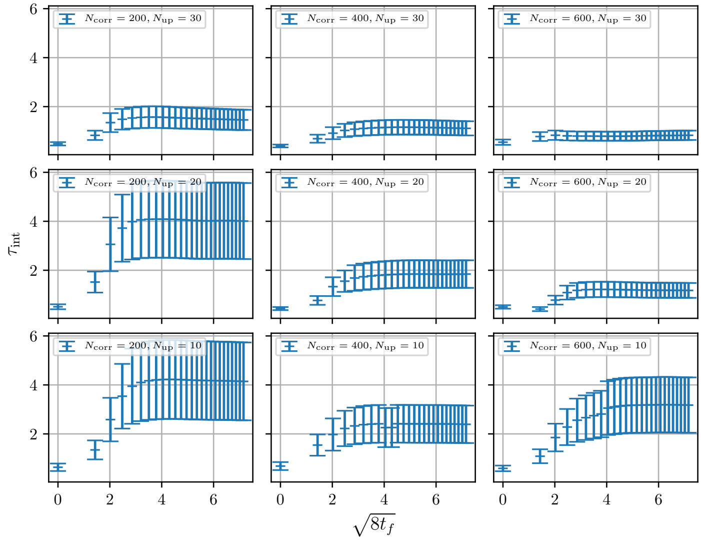
Generated 200 configurations for a lattice of size $N^3 \times N_T = 16^3 \times 32$ and $\beta = 6.0$, for combinations of $N_{\text{corr}} \in [200, 400, 600]$ and $N_{\text{up}} \in [10, 20, 30]$.

- We run for different values for N_{up} and N_{corr} to see what gives optimizes **computational cost** and **autocorrelation**.
- The integrated autocorrelation time for topological charge $\langle Q \rangle$ for a lattice of size $N = 16$ and $N_T = 32$ with $\beta = 6.0$ for combinations of $N_{\text{corr}} \in [200, 400, 600]$ and $N_{\text{up}} \in [10, 20, 30]$, plotted against flow time $\sqrt{8t_f}$.

Optimizing the gauge configuration generation



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- The time taking to generate 200 configurations and flowing them $N_{\text{flow}} = 250$ flow steps for a lattice of size $N = 16$ and $N_T = 32$, with $\beta = 6.0$ for combinations of $N_{\text{corr}} \in [200, 400, 600]$ and $N_{\text{up}} \in [10, 20, 30]$.

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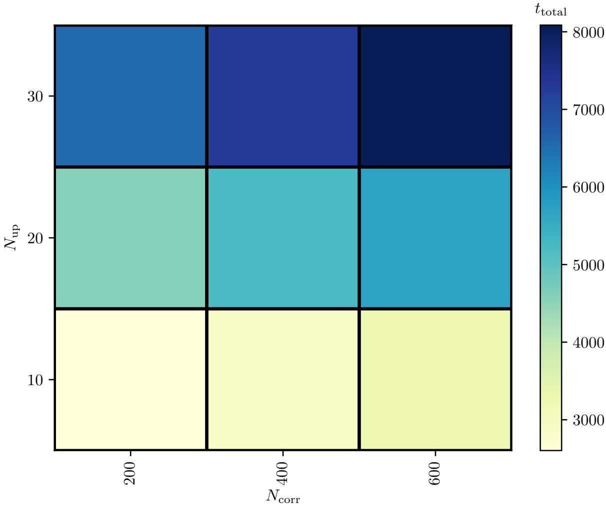

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Gradient flow

The flow equation

The flow of the $\mathrm{SU}(3)$ gauge fields are denoted by $B_\mu(x, t_f)$ which are Lie algebra valued gauge fields,

$$\frac{\mathrm{d}}{\mathrm{d}t_f} B_\mu(x, t_f) = D_\nu \, G_{\nu\,\mu}(x, t_f), \tag{4}$$

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with the initial conditions being the fundamental gauge field,

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

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A bad approximation: *the diffusion equation*,

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

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The smearing radius increases as $\sqrt{8t_f}$.

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- Bad approx.: diffusion equation.
- Topological charge preserved and is more pronounced.
- Renormalizes the topological charge at non-zero flow time.

The flow equation

The flow of the $\mathrm{SU}(3)$ gauge fields are denoted by $B_\mu(x, t_f)$ which are Lie algebra valued gauge fields,

$$\frac{\mathrm{d}}{\mathrm{d}t_f} B_\mu(x, t_f) = D_\nu G_{\nu\,\mu}(x, t_f), \tag{4}$$

$$D_\mu = \partial_\mu + \left[B_\mu(x, t_f), \cdot\right], \tag{5}$$

$$G_{\mu\nu}(x, t_f) = \partial_\mu B_\nu(x, t_f) - \partial_\nu B_\mu(x, t_f) - i[B_\mu(x, t_f), B_\nu(x, t_f)], \tag{6}$$

with the initial conditions being the fundamental gauge field,

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

A bad approximation: *the diffusion equation*,

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

The smearing radius increases as $\sqrt{8t_f}$.

- The flow equation in the continuum is defined by this differential equation.
- With the covariant derivative given by following, with the · being the derivative with respect to flow time.
- The field strength tensor of the flown fields is given in the regular format.
- The initial condition is the un-flowed gauge field, A_μ.
- Bad approx.: diffusion equation.
- Topological charge preserved and is more pronounced.
- Renormalizes the topological charge at non-zero flow time.

Gradient flow on the lattice

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

- On the lattice, the flow equation takes the shape in terms of the link variables.

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with initial condition,

$$V_{t_f}(x,\mu)|_{t_f=0} = U(x,\mu)$$

- On the lattice, the flow equation takes the shape in terms of the link variables.
- Initial conditions similar to the continuum case.

Gradient flow on the lattice

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Note: need to find the action derivative $S_G[V_{t_f}]$.

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- The action derivative is also needed, but that is a minor task we will not cover here.

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Solving gradient flow with Runge-Kutta 3

With

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

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

with coefficients from Lüscher [2].

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Verifying the integration

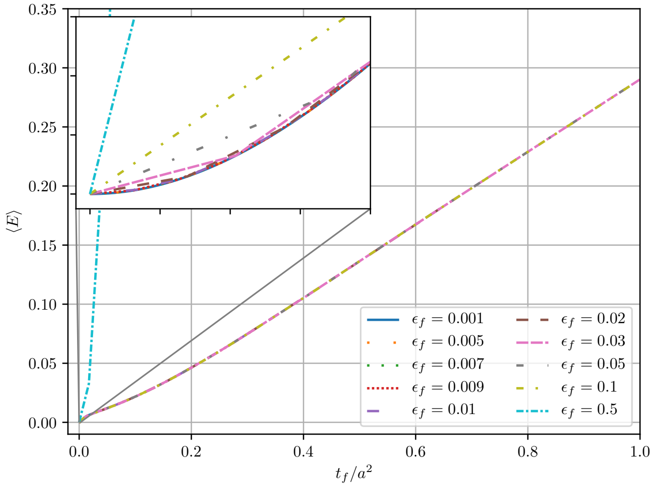
Testing the integrator for different integration steps ϵ_f.

ϵ_f	0.001	0.005	0.007	0.009	0.01	0.02	0.03	0.05	0.1	0.5

- The values we will test the integrator against.

Verifying the integration

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



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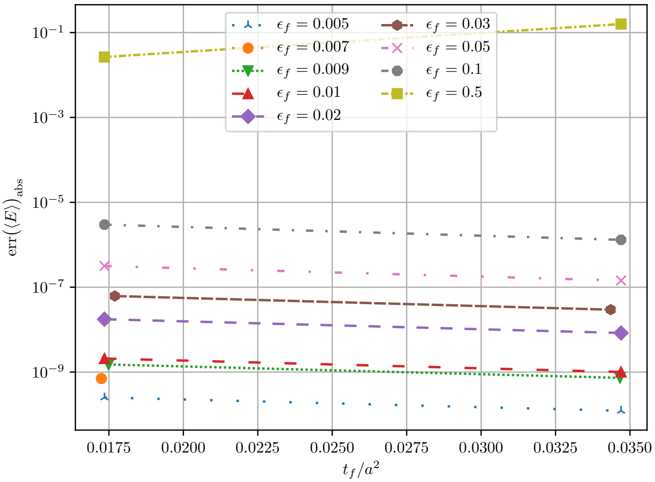
The absolute difference between the smallest flow time $\epsilon_f = 0.001$ and those shown previously.



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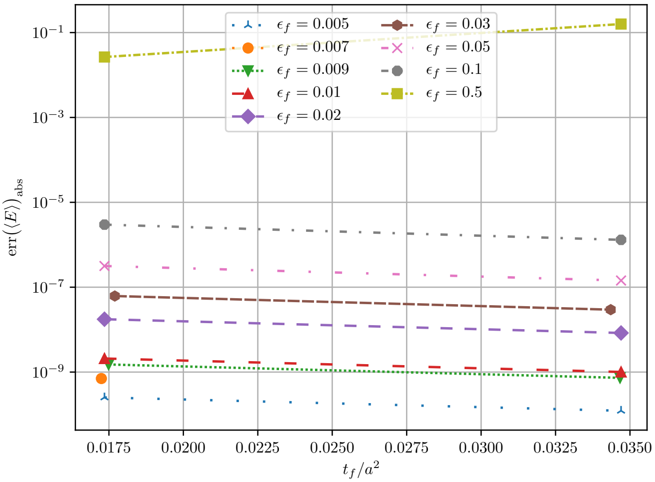

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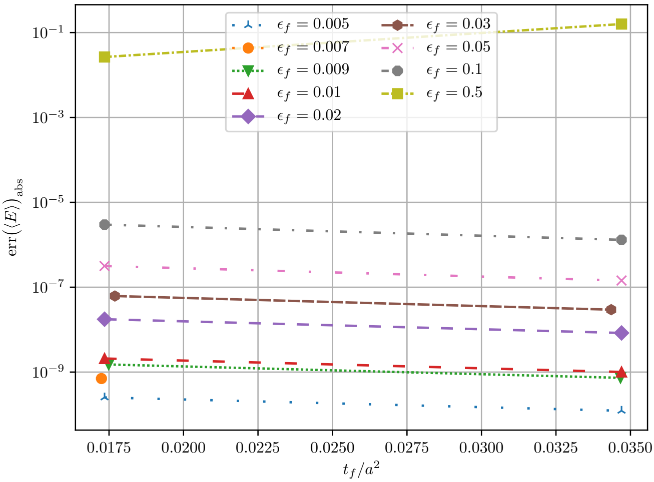

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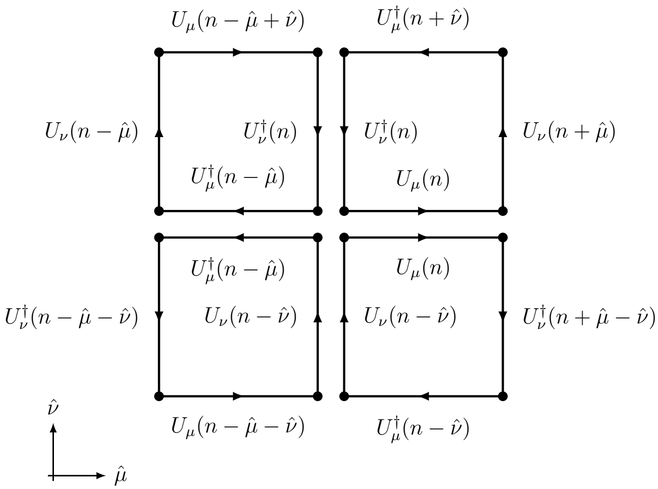
Results

Ensemble	β	N	N_T	N_{cfg}	N_{corr}	N_{up}	ϵ_{flow}	Config. size[GB
A	6.0	24	48	1000	600	30	0.01	0.356
B	6.1	28	56	1000	600	30	0.01	0.659
C	6.2	32	64	2000	600	30	0.01	1.125
D_1	6.45	32	32	1000	1600	30	0.02	0.563
D_2	6.45	48	96	250	1600	30	0.02	5.695

- The main ensembles made for this thesis.
- Every configuration was flown with $N_{\mathrm{flow}} = 1000$ flow steps.
- We should also mention that we generated a few additional ensembles for investigating other aspects of the topological charge.

The clover field strength definition



- We will use the clover field strength definition in gauge observables.

Energy definition

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

- We can use this definition to set a scale.

Energy definition

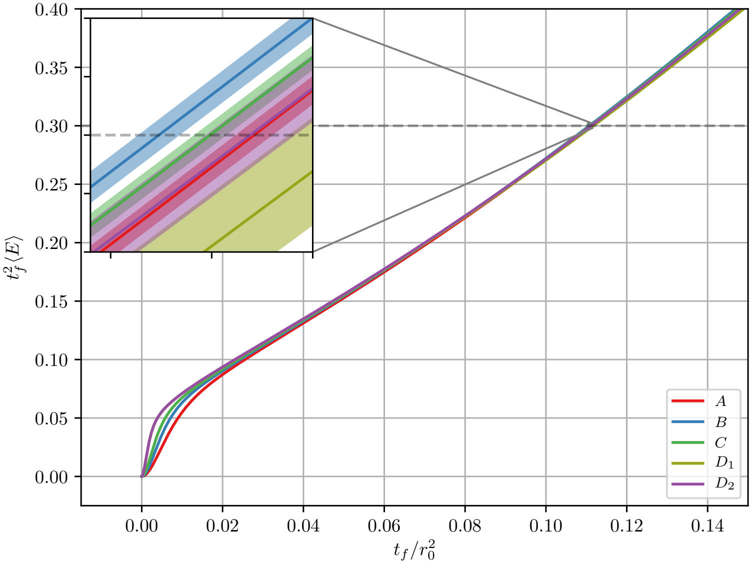
$$E = \frac{a^4}{2|\Lambda|} \sum_{n \in \Lambda} \sum_{\mu,\nu} \left(F^{\mathrm{clov}}_{\mu\nu}(n) \right)^2$$

We can use this definition to set a scale t_0,

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

- We can use this definition to set a scale.

Energy



0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
$t_f^2 \langle E \rangle$
0.00
0.02
0.04
0.06
0.08
0.10
0.12
0.14
t_f / r_0^2
A
B
C
D_1
D_2

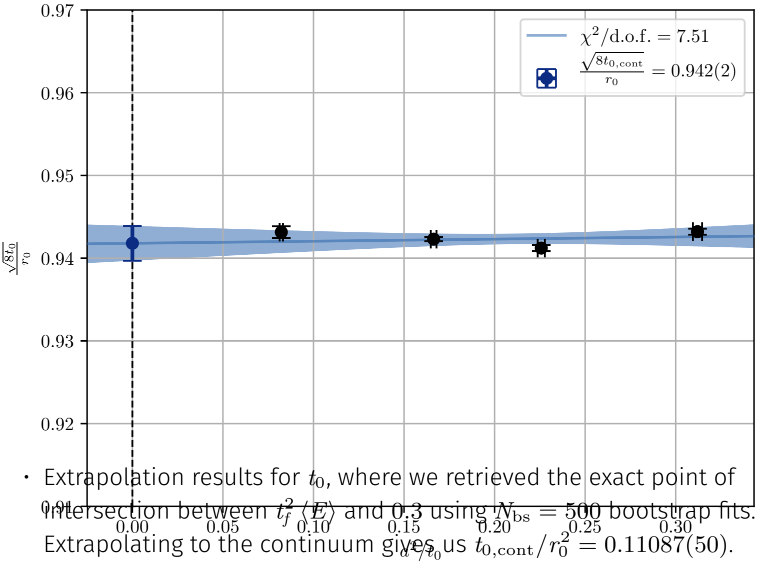
Scale setting t_0

Ensemble	$t_0[\text{fm}^2]$	t_0/a^2	t_0/r_0^2	L/a	L [fm]	a [f
A	$0.02780(2)$	$3.20(3)$	$0.11121(9)$	24	$2.235(9)$	$0.0931($
B	$0.02769(2)$	$4.43(4)$	$0.11075(10)$	28	$2.214(10)$	$0.0791($
C	$0.02775(2)$	$6.01(6)$	$0.11099(8)$	32	$2.17(1)$	$0.0679($
D_1	$0.02779(5)$	$12.2(1)$	$0.1112(2)$	32	$1.530(9)$	$0.0478($
D_2	$0.02794(9)$	$12.2(1)$	$0.1117(3)$	48	$2.29(1)$	$0.0478($

- Extrapolation results for t_0, where we retrieved the exact point of intersection between $t_f^2 \langle E \rangle$ and 0.3 using $N_{\text{bs}} = 500$ bootstrap fits. Extrapolating to the continuum gives us $t_{0,\text{cont}}/r_0^2 = 0.11087(50)$.

Scale setting t_0

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



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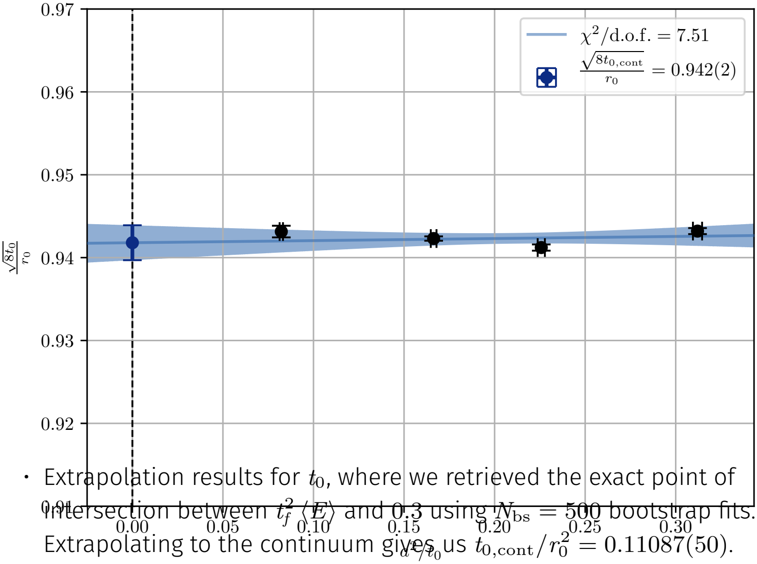

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- $r_0 = 0.5$ fm.

Scale setting t_0

This matches the values retrieved by Lüscher [2].

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- The continuum extrapolation $a \to 0$ for t_0 of the four ensembles A, B, C, and D_2.
- $r_0 = 0.5$ fm.

Scale setting w_0

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

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

Scale setting w_0

Autocorrelation in the energy

Topological charge definition

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

with the charge density given by

$$q(n) = \frac{1}{32\pi^2} \epsilon_{\mu\nu\rho\sigma} \mathrm{tr}\left[F_{\mu\nu}(n) F_{\rho\sigma}(n)\right].$$

- We will use the clover field strength definition.
- Symmetries will allow us to reduce the effective number of clovers need to calculate from 24 to 6.

Topological charge

Topological charge autocorrelation

Topological susceptibility

The fourth cumulant

The effective glueball mass

Conclusion

Questions?

References

[1] Hilmar Forkel. A Primer on Instantons in QCD. *arXiv:hep-ph/0009136*, September 2000. URL `http://arxiv.org/abs/hep-ph/0009136`. arXiv: hep-ph/0009136.

[2] 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.