

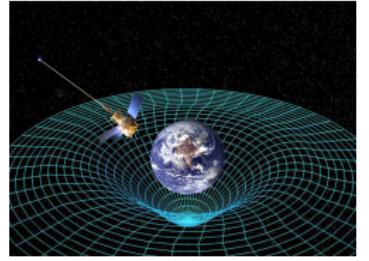
Solving SU3 Yang-Mills theory on the lattice: a calculation of selected gauge observables with gradient flow

Hans Mathias Mamen Vege
04.07.19

Supervisor: *Andrea Shindler*
Co-supervisor: *Morten Hjorth-Jensen*

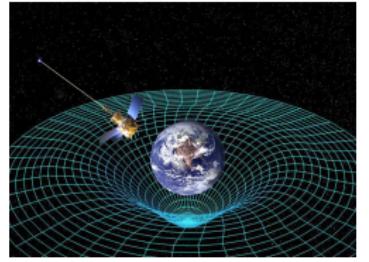
University of Oslo

The four forces of nature



Gravity

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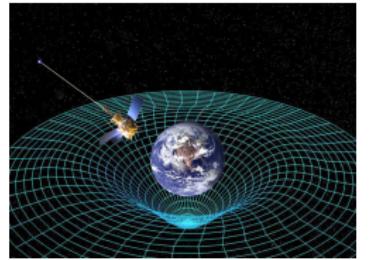


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Electromagnetism

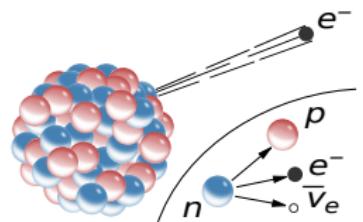
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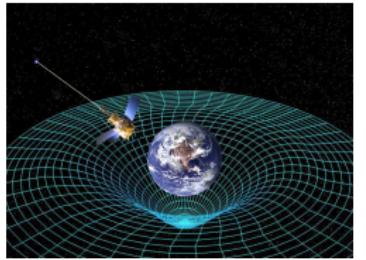


Electromagnetism



Weak nuclear force

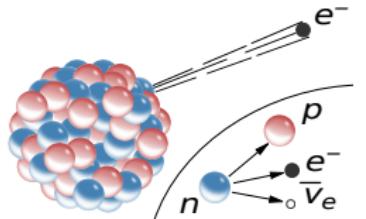
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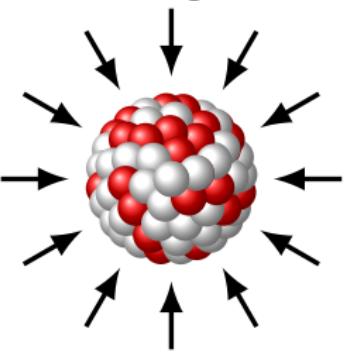
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Strong nuclear force

What is the strong force?

Consists of:

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

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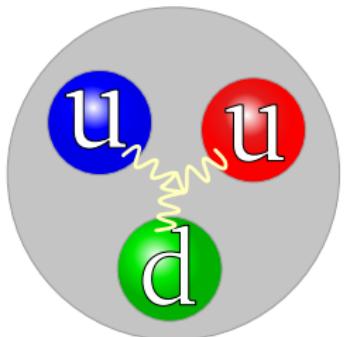
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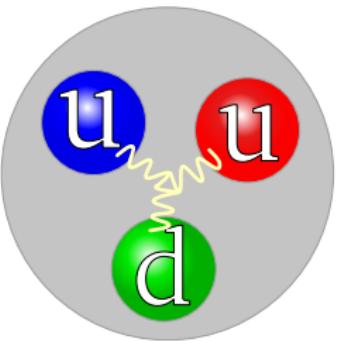
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Mass discrepancy:

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

$$936 \text{ MeV} \neq 3 \text{ MeV} + 3 \text{ MeV} + 6 \text{ MeV}.$$



Comparing the strong force and QED

QED Quantum Electrodynamics(Electromagnetism):

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

Field strength tensor:

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The strong nuclear force, QCD:

$$\mathcal{L}_{\text{QCD}} = \sum_{f=u,d,\dots} \bar{\psi}_f (i\gamma^\mu (\partial_\mu + ig_S A_\mu^a T^a) - m_f) \psi_f - \frac{1}{4} F_{\mu\nu}^a F^{a\mu\nu}$$

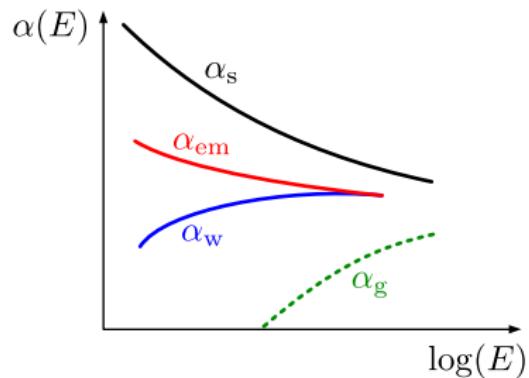
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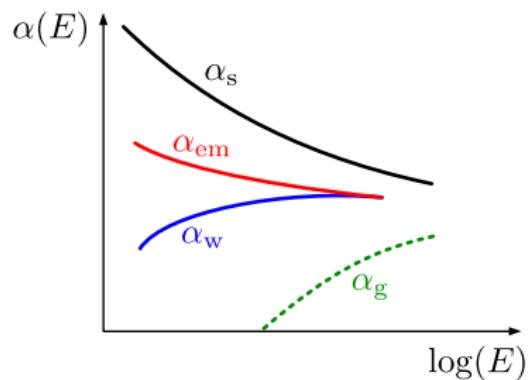
Why is the strong force strong?

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Coupling constant α strength of the force in an interaction.



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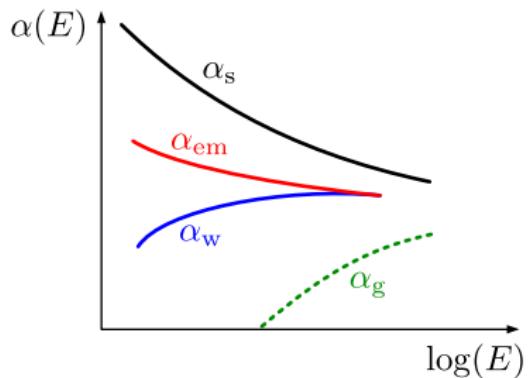


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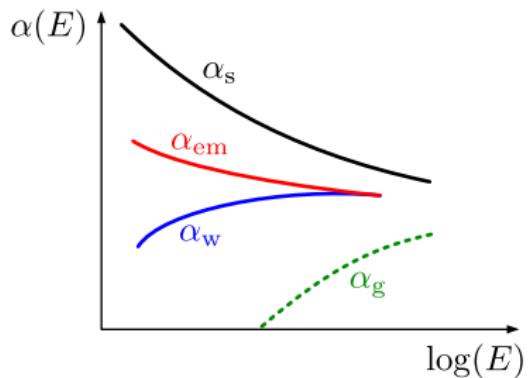


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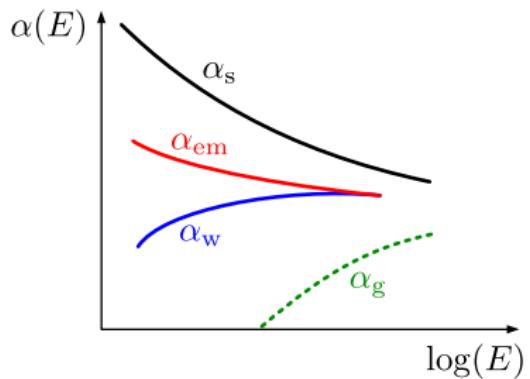


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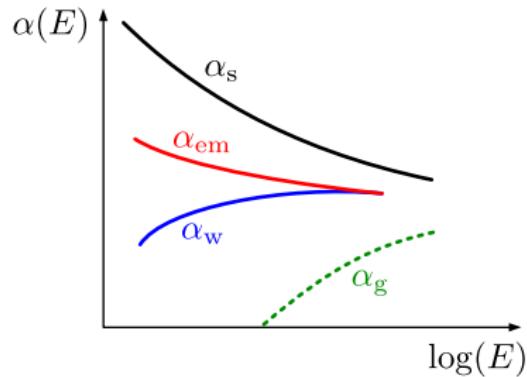


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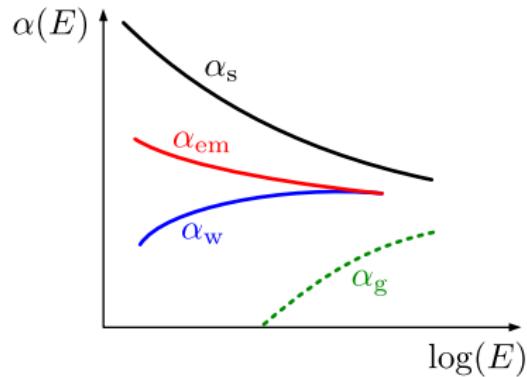
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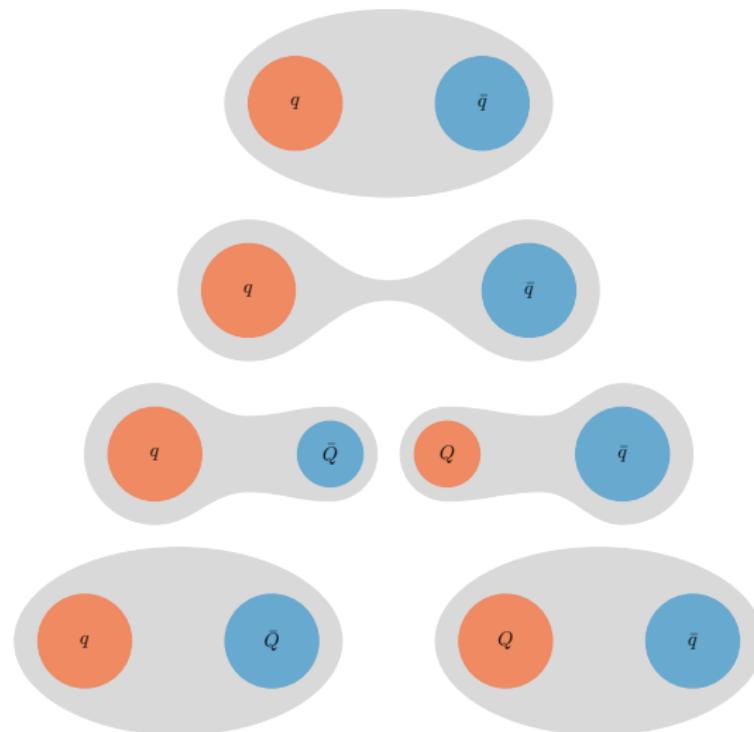
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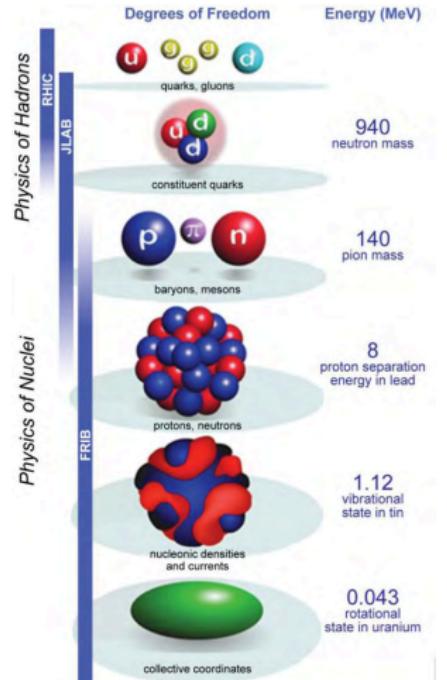
Confinement: a low-energy phenomena

No free color charges in nature!



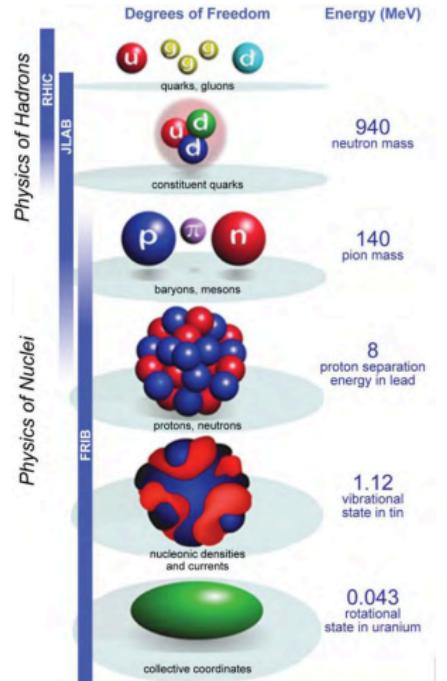
If we try to pull apart **two quarks in a meson**, more and more energy is required until we have enough energy to spontaneously create a **quark-antiquark pair**, forming thus **two new mesons**.

QCD and nuclear physics



Need to understand the
low-energy regime in order to
better understand nuclear
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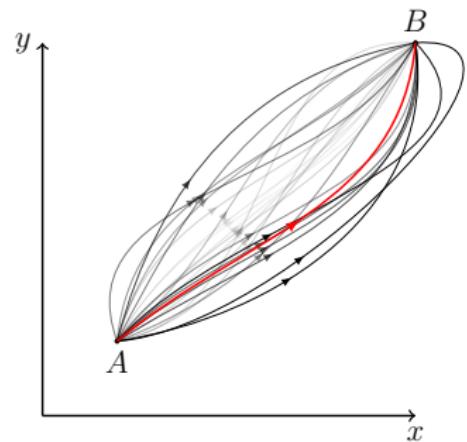
QCD and nuclear physics



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→ numerical methods(e.g. lattice QCD)

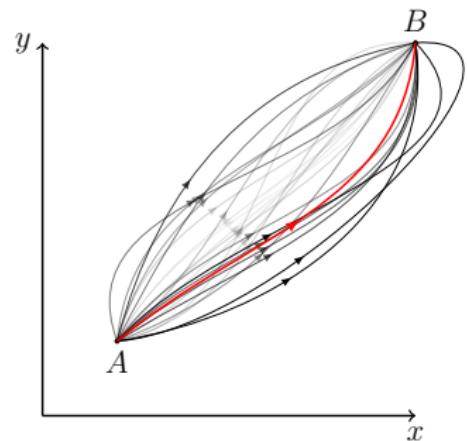
How we measure: path integrals

Sum over all possible paths → the most likely path.



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Principle of least action (or stationary condition): $\frac{\delta}{\delta x(t)} (S [x(t)]) = 0$

Given a field ϕ^M in Minkowski space, the *partition function* Z is given by

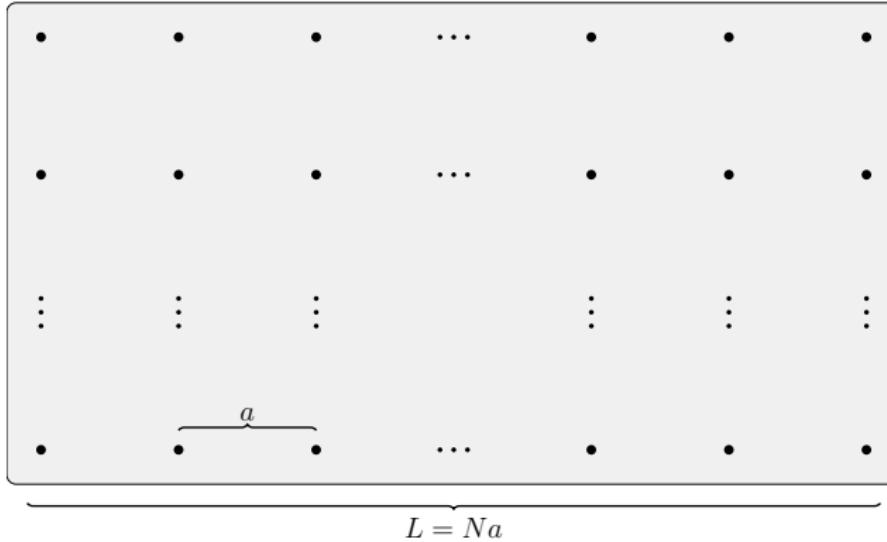
$$\begin{aligned} Z &= \int \mathcal{D}[\phi^M] e^{\frac{i}{\hbar} S^M[\phi^M]} \\ &\downarrow \quad \hbar = 1, \quad \tau \rightarrow -it \quad \text{imaginary time!} \\ &= \int \mathcal{D}[\phi] e^{-S[\phi]} \end{aligned}$$

where \mathcal{D} is an integration of all possible paths in space.

An observable O becomes,

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

Discretizing the path integral



Discretizing the path integral

Path integral integration measure becomes

$$\int \mathcal{D}\phi = \prod_{x_\mu} d\phi(x) = \prod_{x_\mu} d\phi_{x_\mu}$$

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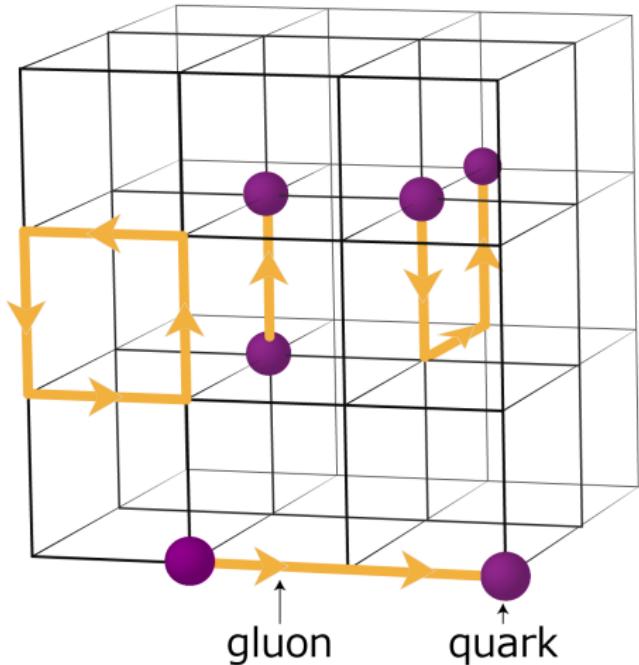
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- Quarks in points, gluons in-between (links).
- The lattice is a cube in 4D.
- Maintains the SU(3) symmetry by introducing links.
- Paths of links with fermions as end points are gauge invariant.
- Closed loops are gauge invariant.

We exclude fermions to only look at the gauge fields,

$$S_G = \frac{1}{2} \int d^4x \text{tr} (F_{\mu\nu})^2$$

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$$U_\mu^\dagger(x) = U_\mu^{-1}(x), \quad \det(U_\mu(x)) = 1.$$

Parallelization: distributing the problem

Number of points in a lattice:

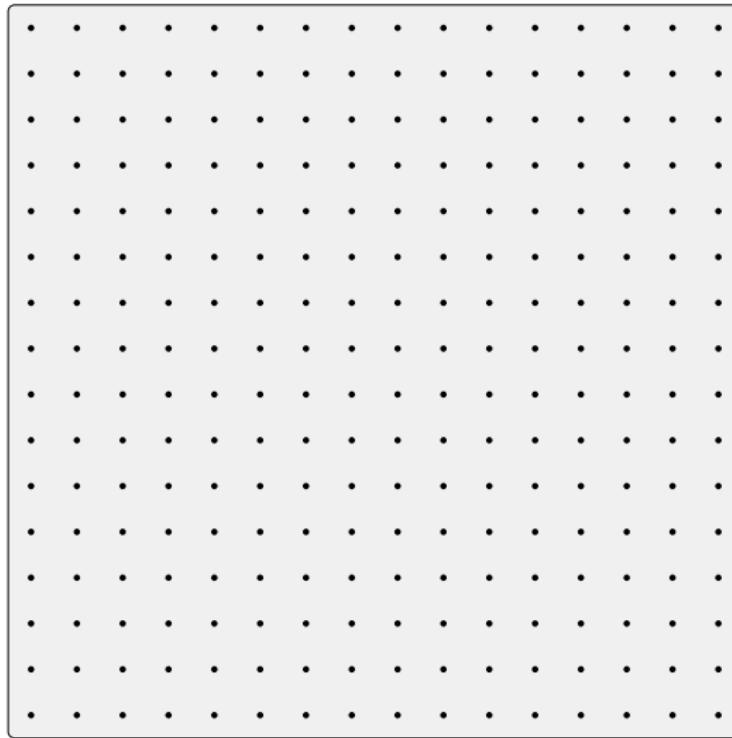
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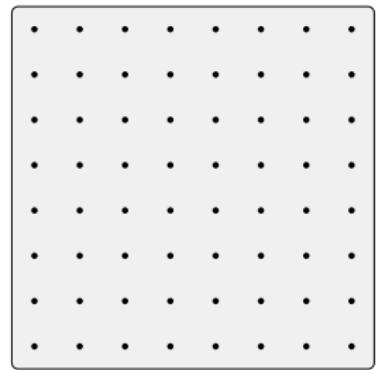
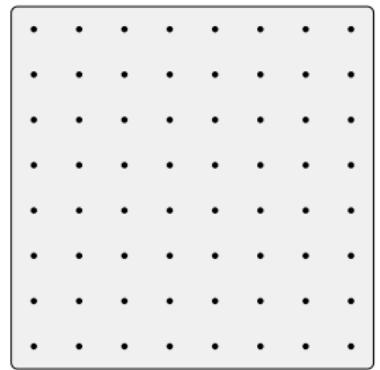
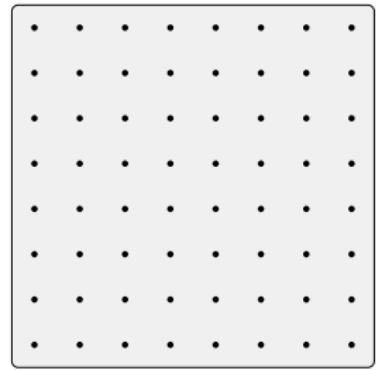
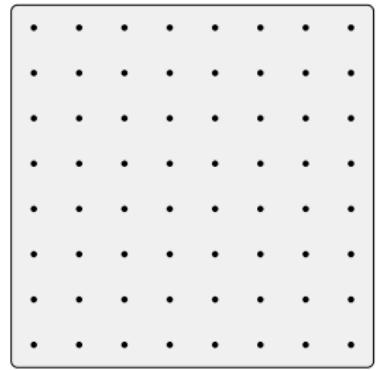
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Too large to solve on any single computer

Parallelization: splitting the hypercube



Parallelization: splitting the hypercube



Parallelization: shifts

Communications between nodes set up with MPI.

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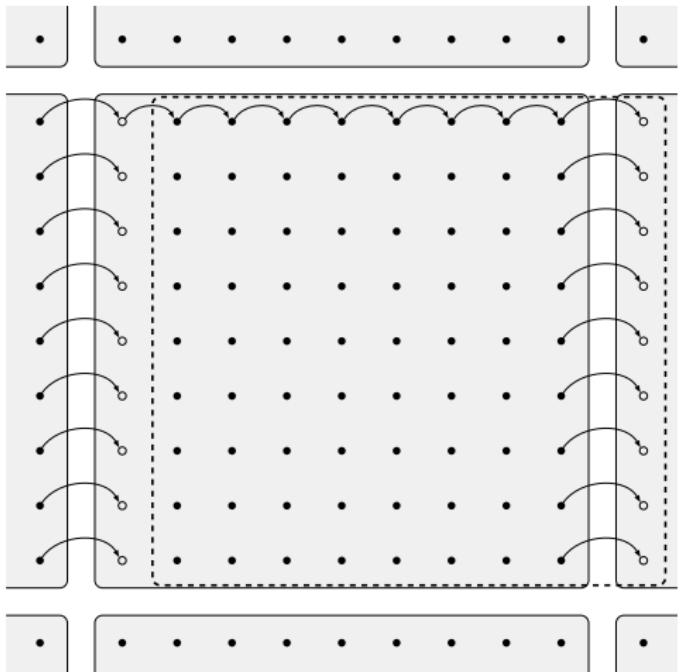
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$$B_\mu(x, t_f) \Big|_{t_f=0} = A_\mu(x)$$

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An analogy: the diffusion equation:

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

¹Lüscher [3]

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Solve on the lattice using the symplectic, structure preserving
Runge-Kutta 3 generator²

²Munthe-Kaas [4]

Results

Ensembles

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

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

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

Lattice sizes

The lattice sizes.

Ensemble	N	$L = Na$ [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)

Charge radius of a proton: ~ 0.85 fm.

Energy definition

- Defined as the field strength tensor squared averaged over all lattice points and directions.
- We can use this definition to set a scale.

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

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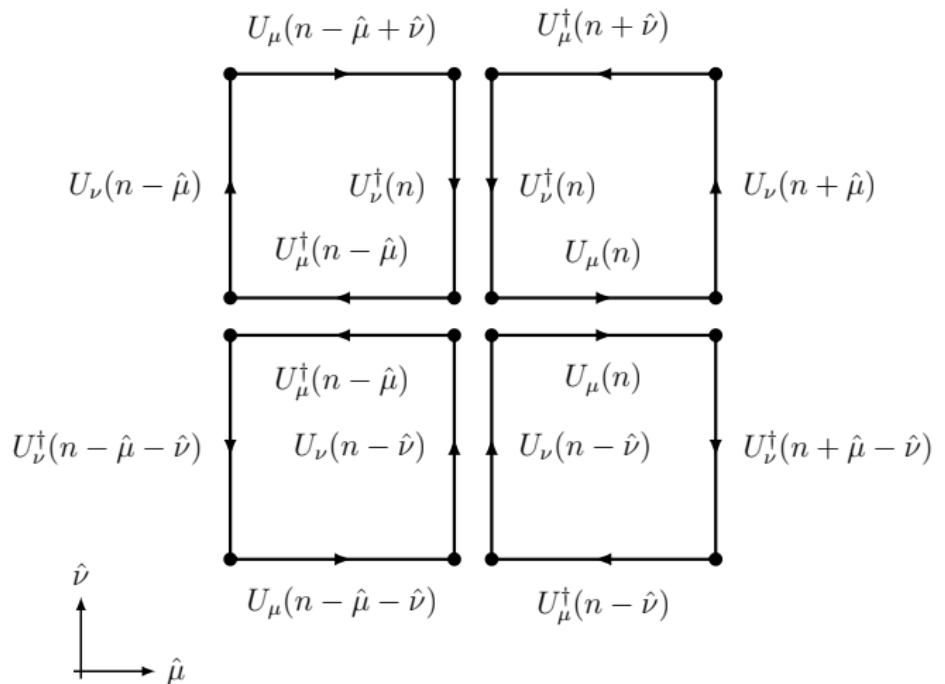
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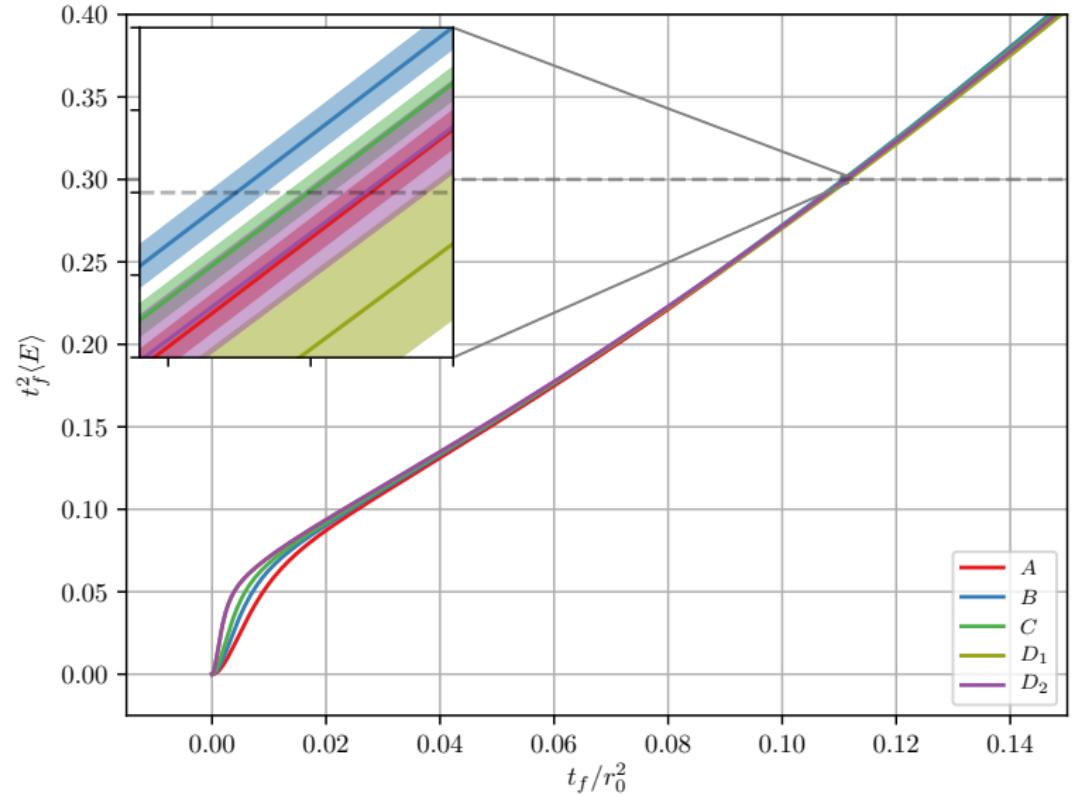
$$\left\{ t_f^2 \langle E(t) \rangle \right\}_{t_f=t_0} = 0.3.$$

The clover field strength definition

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

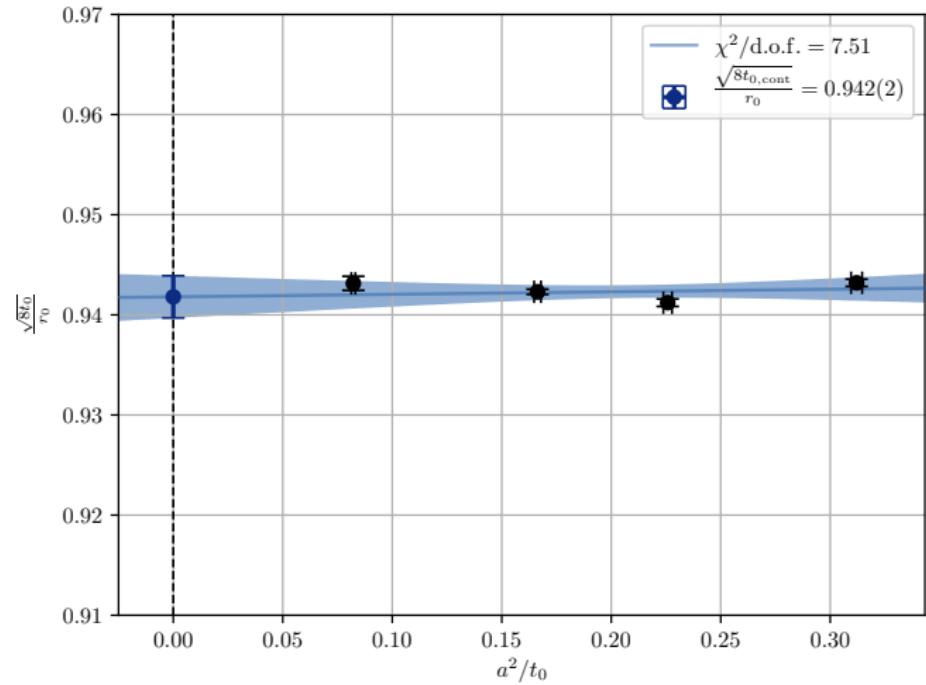


- We will use the clover field strength definition in gauge observables.
- **Symmetries** will allow us to **reduce** the effective **number of clovers** need to **calculate from 24 to 6**.

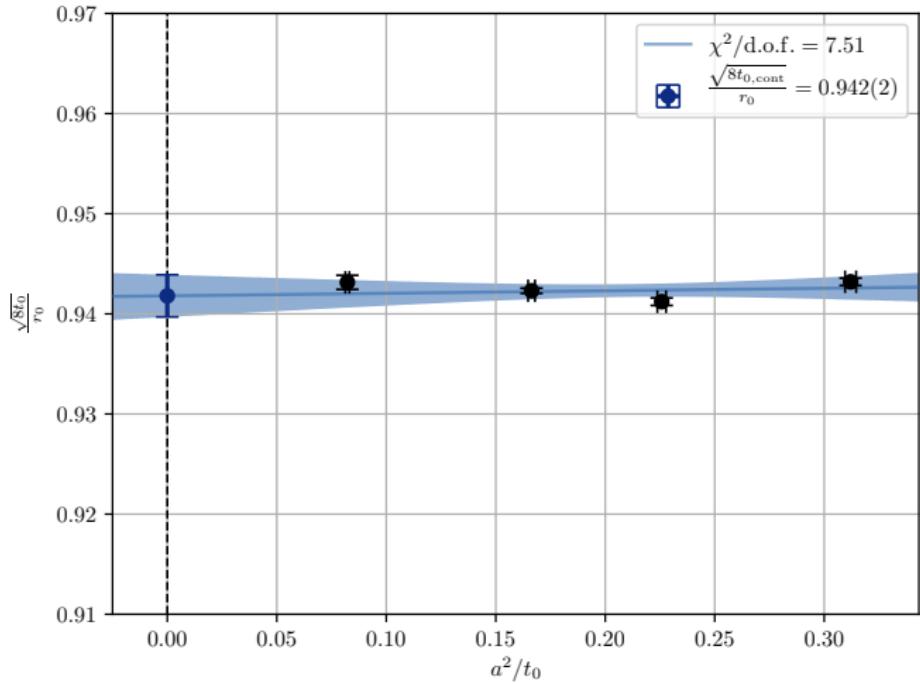


Scale setting t_0

- The continuum extrapolation $a \rightarrow 0$ for t_0 of the four ensembles A , B , C , and D_2 .



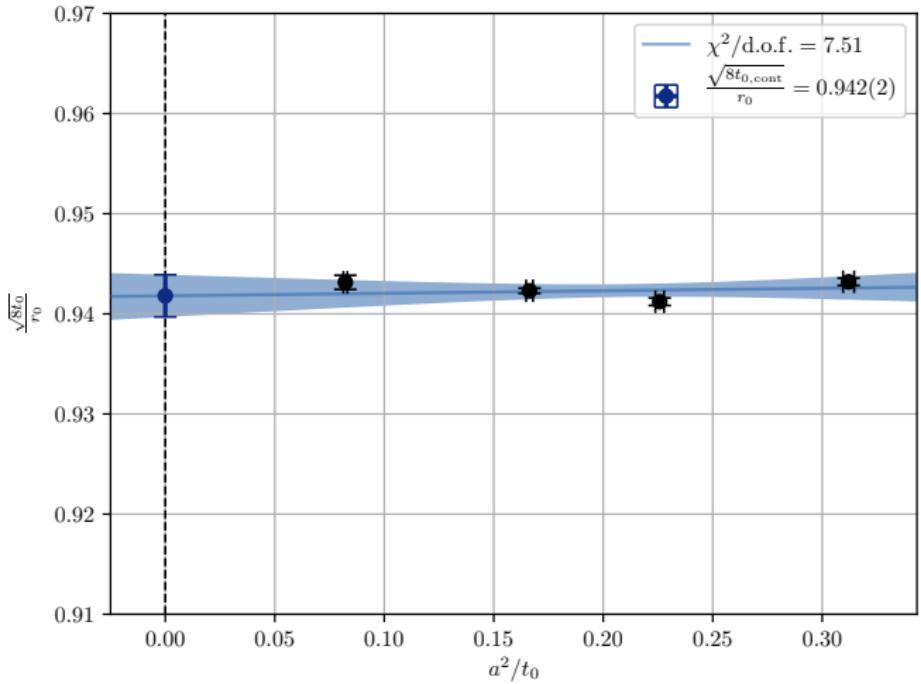
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Continuum extrapolation using ensembles A , B , C , and D_2 gives
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Scale setting t_0

- Notice the $\chi^2/\text{d.o.f.}$ of the extrapolation versus the two other extrapolations.

Extrapolations for different ensemble-combinations

Ensembles	$t_{0,\text{cont}}/r_0^2$	$\chi^2/\text{d.o.f.}$
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,

$$W(t)|_{t=w_0^2} = 0.3,$$

$$W(t) \equiv t_f \frac{d}{dt_f} \left\{ t_f^2 \langle E \rangle \right\}.$$

First presented by Borsanyi et al. [1].

Scale setting w_0

Ensembles	$w_{0,\text{cont}}[\text{fm}]$	$\chi^2/\text{d.o.f}$
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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Comparable to Borsanyi et al. [1] which included dynamical fermions,
with $w_{0,\text{cont}} = 0.1755(18)(04)$ fm.

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- Can in a very crude manner be viewed as the “curl” of the gauge fields.

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with the charge density given by

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

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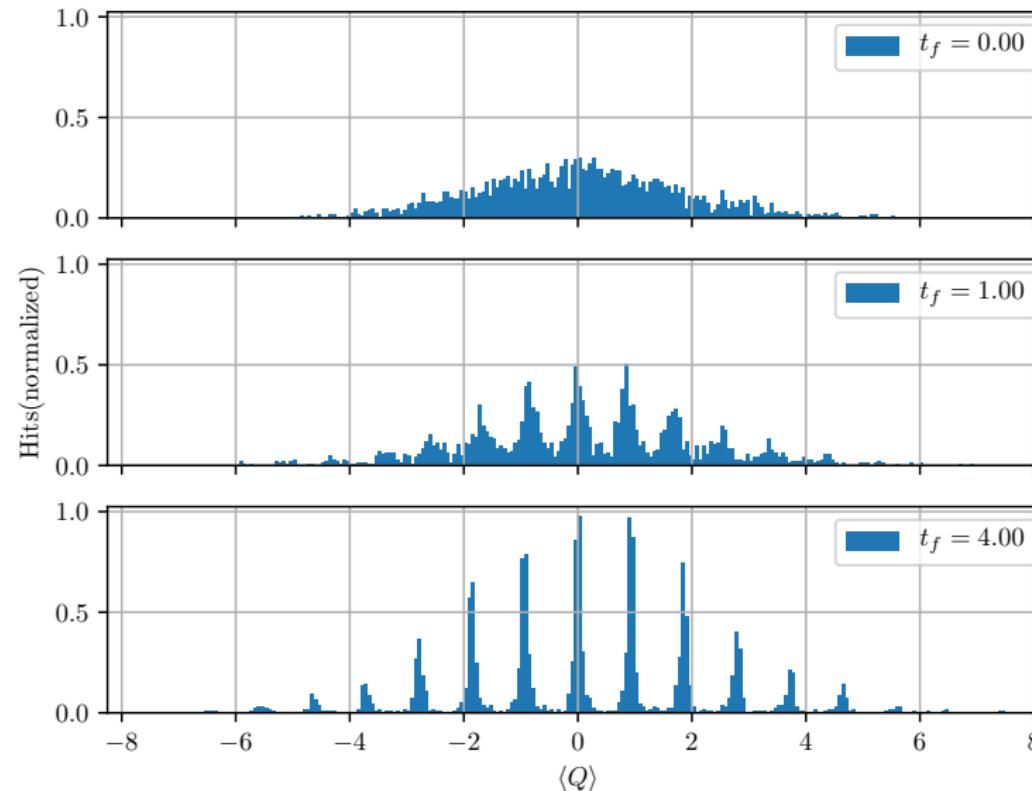
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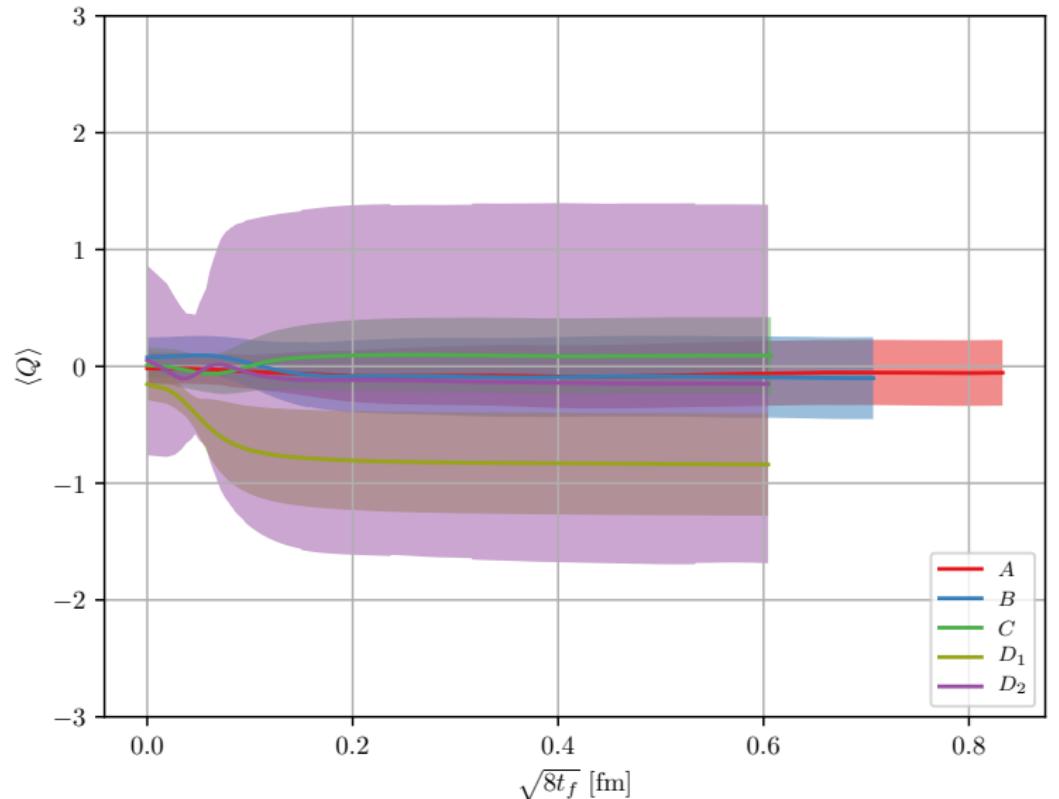
Topological charge

Topological charge distribution

Histograms for the Q for ensemble G with a lattice of size $N^3 \times N_T = 16^3 \times 32$ with $\beta = 6.1$, taken at different flow times $t_f/a^2 = 0.0, 1.0, 4.0$ fm.



Topological charge for our main ensembles

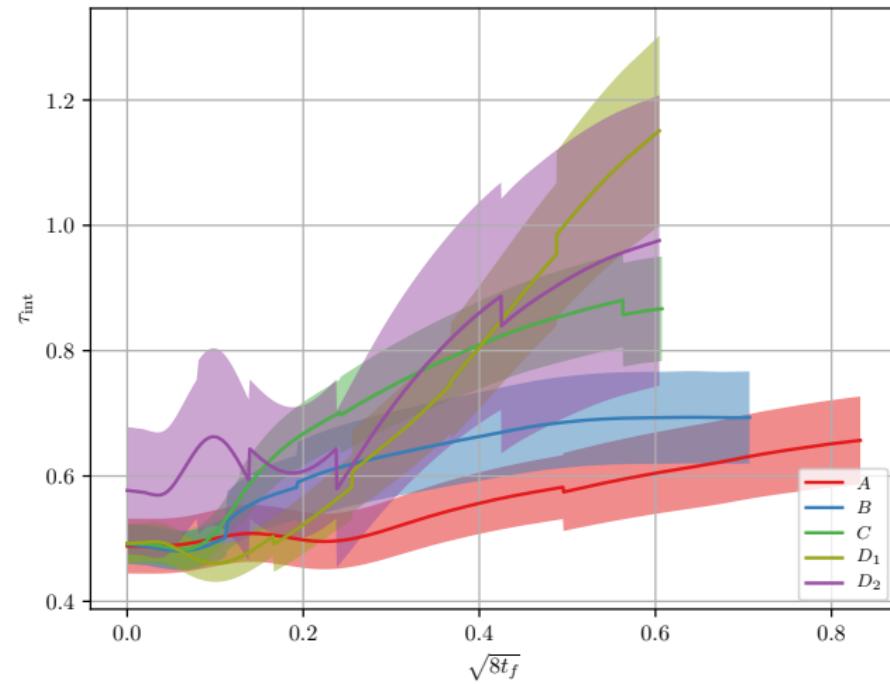


First of all, Q is a far more correlated than other quantities such as the energy.

Why is the charge not centered around zero for certain ensembles?

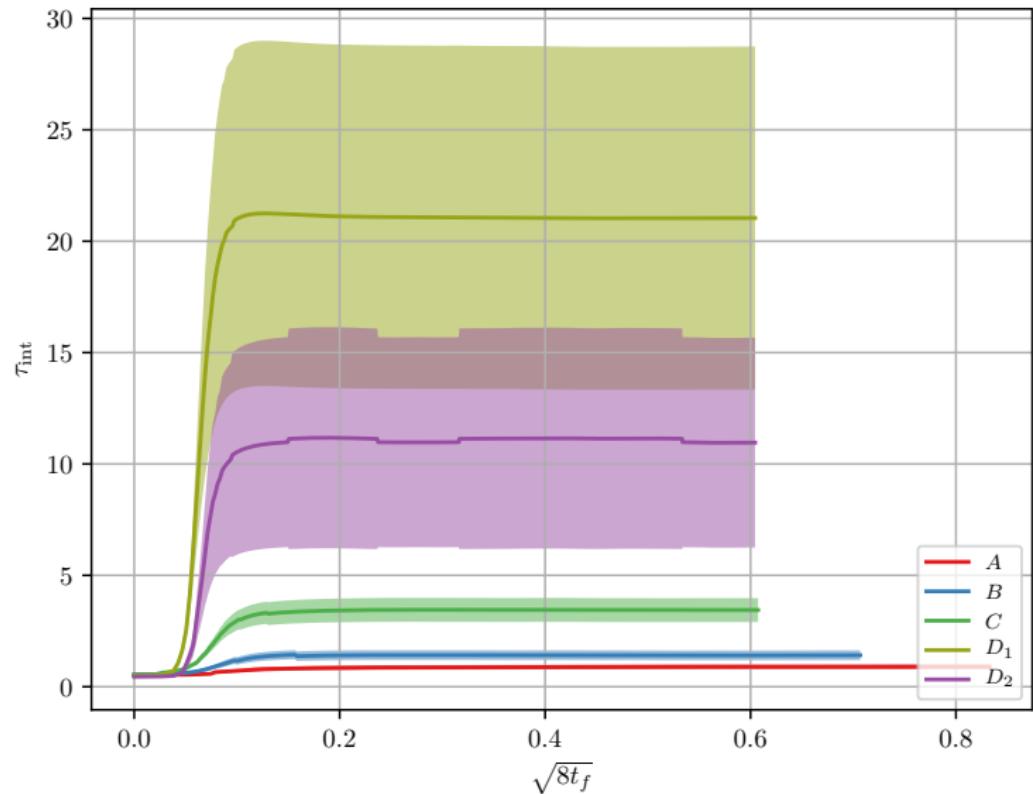
Autocorrelation in the energy

The autocorrelation of the energy. A value of $\tau_{\text{int}} = 0.5$ indicates that we have zero autocorrelation.



Topological charge autocorrelation

- The integrated autocorrelation τ_{int} for topological charge for the five main ensembles.



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

with V being the lattice volume and $\langle Q^2 \rangle$ is the second momenta of the charge.

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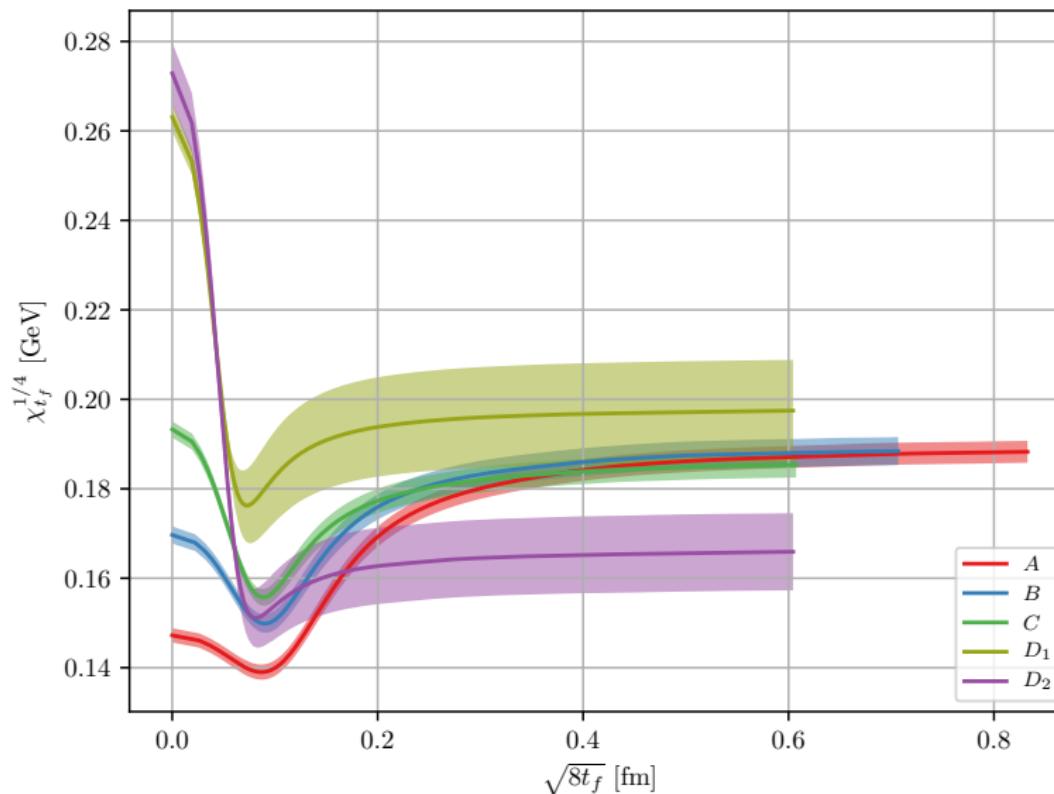
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Topological susceptibility



- The topological susceptibility $\chi_{tf}^{1/4}$ of the **main ensembles**.
- We have a **UV divergence at zeroth flow time**, hence to need for gradient flow which renormalizes this quantity.
- **Bootstrapped** $N_{\text{bs}} = 500$ times.
- Corrected for autocorrelations with $\sigma = \sqrt{2\tau_{\text{int}}}\sigma_0$.

Topological susceptibility continuum extrapolation

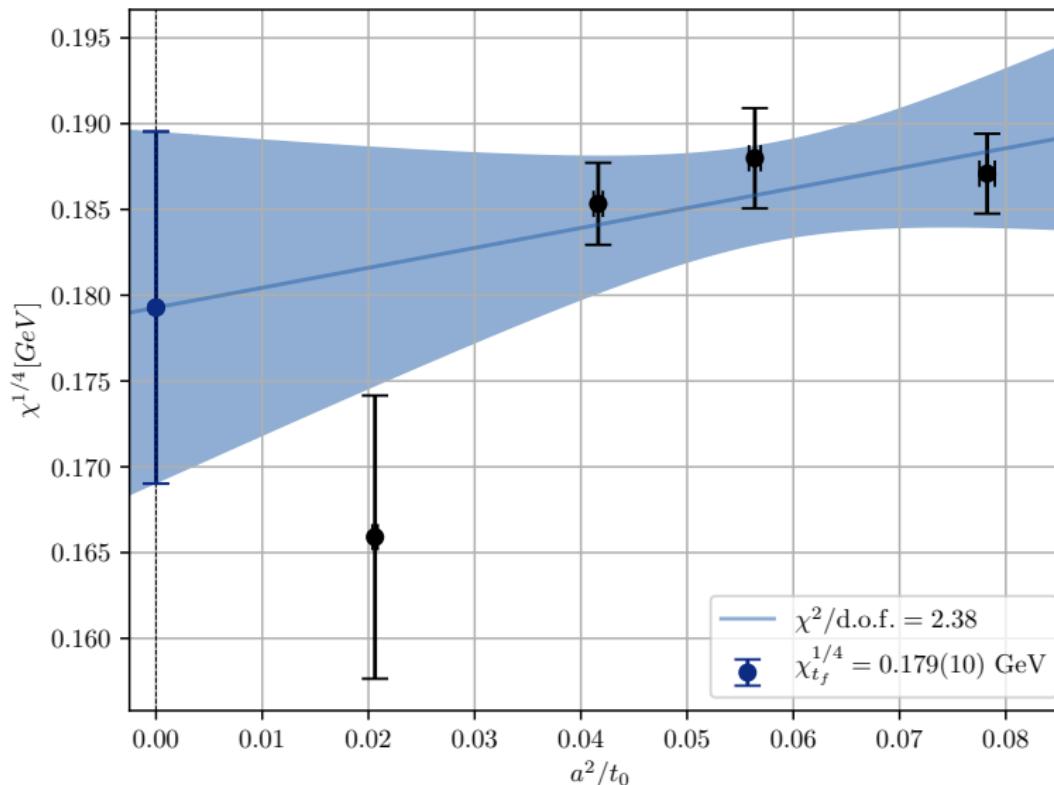
Ensemble	$\chi_{t_f}^{1/4}$ [GeV]	$\chi_{t_f}^{1/4}$ [GeV], corrected	$\sqrt{2\tau_{\text{int}}}$
<i>A</i>	0.1877(23)	0.1877(24)	1.028(46)
<i>B</i>	0.1880(21)	0.1880(29)	1.346(81)
<i>C</i>	0.1853(14)	0.1853(24)	1.762(104)
<i>D</i> ₁	0.1971(22)	0.1971(101)	4.523(675)
<i>D</i> ₂	0.1656(33)	0.1656(86)	2.624(441)

Error corrected for autocorrelations with $\sigma = \sqrt{2\tau_{\text{int}}}\sigma_0$.

Values taken at $\sqrt{8t_f} = 0.6$ fm.

- Values extracted at a smearing radius of **hadronic scales**. That is, we have plateaued and have no discretization effects.
- The topological susceptibility for the main ensembles together with the correction factor from the integrated autocorrelation time. The second column have not had its results corrected by $\sqrt{2\tau_{\text{int}}}$. None of the results have been analyzed with bootstrapping.

Topological susceptibility continuum extrapolation



- A continuum extrapolation of the topological susceptibility $\chi_{tf}^{1/4}$ for the main ensembles excluding the D_1 ensemble.
- The points for $\chi_{tf}^{1/4}$ is taken at $\sqrt{8t_{f,0}} = 0.6 \text{ fm}$.

Ensembles	$\chi_{tf}^{1/4} (\langle Q^2 \rangle) [\text{GeV}]$	N_f	$\chi^2/\text{d.o.f}$
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
B, C, D_1	0.187(24)	3.18(24)	1.63
B, C, D_2	0.166(24)	5.06(39)	2.05
A, B, C	0.184(6)	3.37(26)	0.33

The fourth cumulant

- Highly unstable, as we shall see.
- Will provide insight into the goodness of our ensembles.
- An R -value away from 1 will indicate that QCD cannot be described by the dilute instanton gas model.

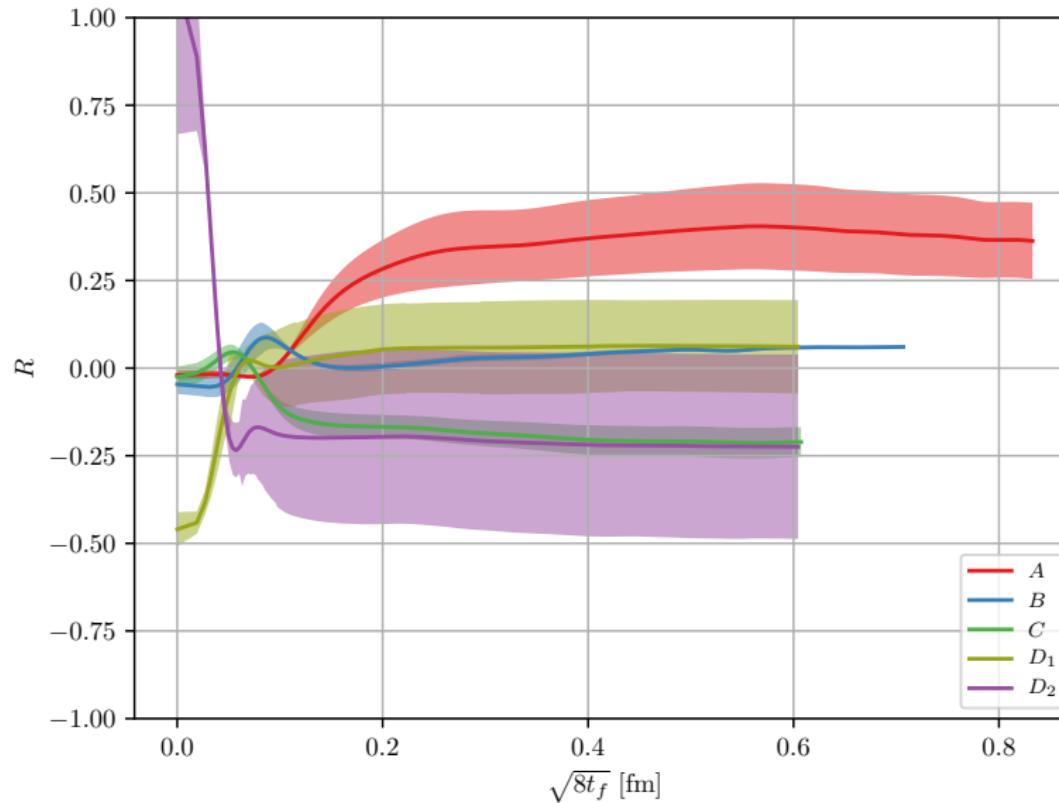
$$\langle Q^4 \rangle_c = \frac{1}{V^2} \left(\langle Q^4 \rangle - 3 \langle Q^2 \rangle^2 \right).$$

From this, we can also measure the ratio R ,

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

The fourth cumulant

- The fourth cumulant ratio $R = \langle Q^4 \rangle_C / \langle Q^2 \rangle$.
- The results was analyzed using $N_{\text{bs}} = 500$ bootstrap samples, with the error corrected for by $\sqrt{2\tau_{\text{int}}}$.



The fourth cumulant at reference flow times

The fourth cumulant is taken at their individual reference scales seen in the third column. The data were analyzed with using a bootstrap analysis of $N_{bs} = 500$ samples, with error corrected by the integrated autocorrelation, $\sqrt{2\tau_{int}}$.

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. [2]

Comparing fourth cumulant

- Parameters of the ensembles presented by Cè et al. [2]. The first column is the ensemble name from the article. The letter indicates the volume, while the subindex indicates the β value. Ensembles of similar letters keep approximately the same length L .

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

- Results as presented by Cè et al. [2], **normalized by the lattice volume.**

Ensemble	$\langle Q^2 \rangle_{\text{normed}}$	$\langle Q^4 \rangle_{\text{normed}}$	$\langle Q^4 \rangle_{C,\text{normed}}$	R_{normed}
F_1	0.728(1)	1.608(4)	0.016(1)	0.022(1)
B_2	0.772(3)	1.873(19)	0.085(4)	0.110(5)
\tilde{D}_2	0.770(3)	1.817(17)	0.037(4)	0.048(5)
B_3	0.760(3)	1.805(17)	0.074(3)	0.097(4)
\tilde{D}_3	0.769(3)	1.801(14)	0.027(1)	0.035(1)
B_4	0.776(3)	1.874(18)	0.069(3)	0.089(4)
\tilde{D}_4	0.785(3)	1.891(17)	0.040(4)	0.052(5)

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)

- A comparison between the results obtained in this thesis on the fourth cumulant, and by those similar in volume form Cè et al. [2]. *Ratio* indicates that we are dividing our results by the ones in previous table.

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- $q(0)$ is not required to be at $n_t = 0$.

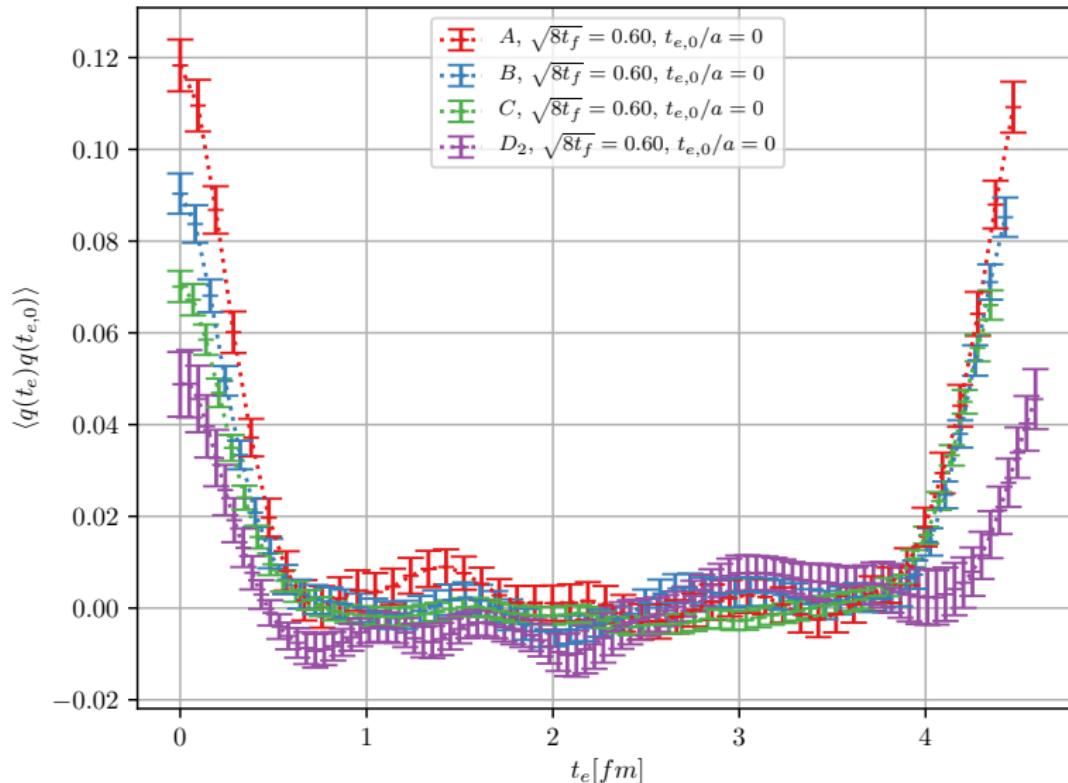
The **topological charge correlator**

$$C(n_t) = \langle q(n_t)q(0) \rangle,$$

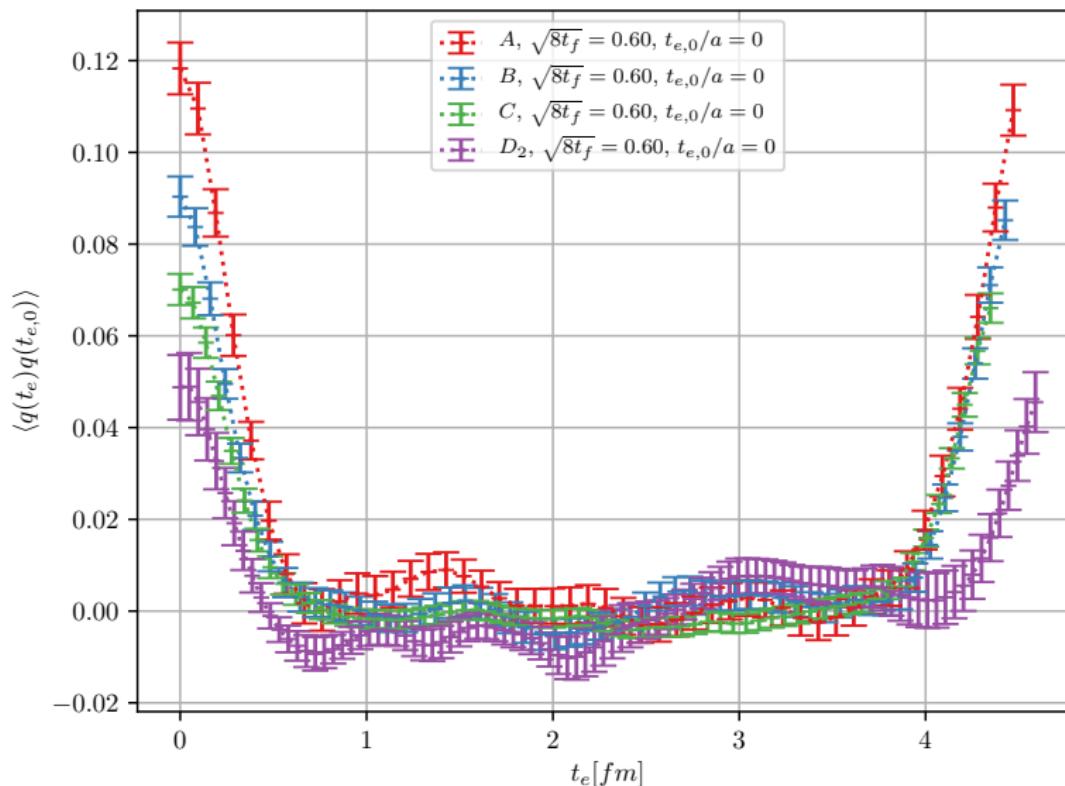
$q(0)$ is the *source* placed at a fixed Euclidean time, and $q(n_t)$ is the *sink* which is summed across all Euclidean times.

The topological charge correlator

- The topological charge correlator for all of the ensembles except D_1 . The x -axis contains the sink-source separation, as the source $q(0)$ is placed at $t_e = 0$ fm, and the sink $q(t_e)$ is taken at t_e .

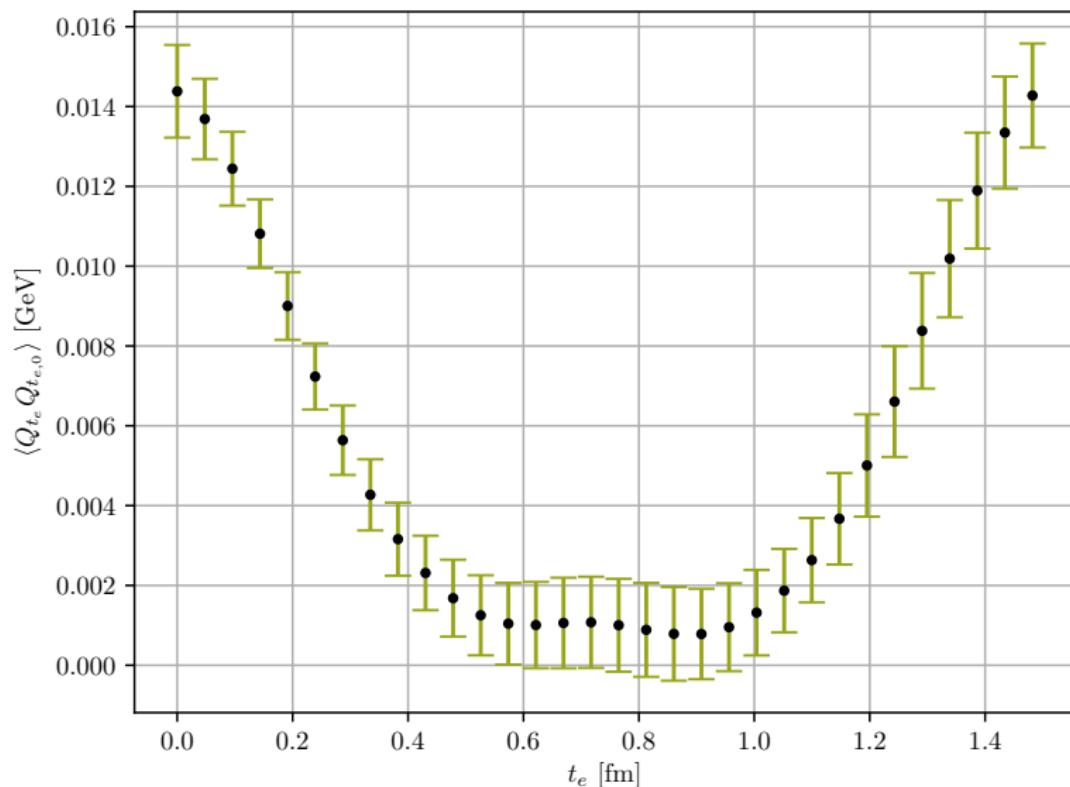


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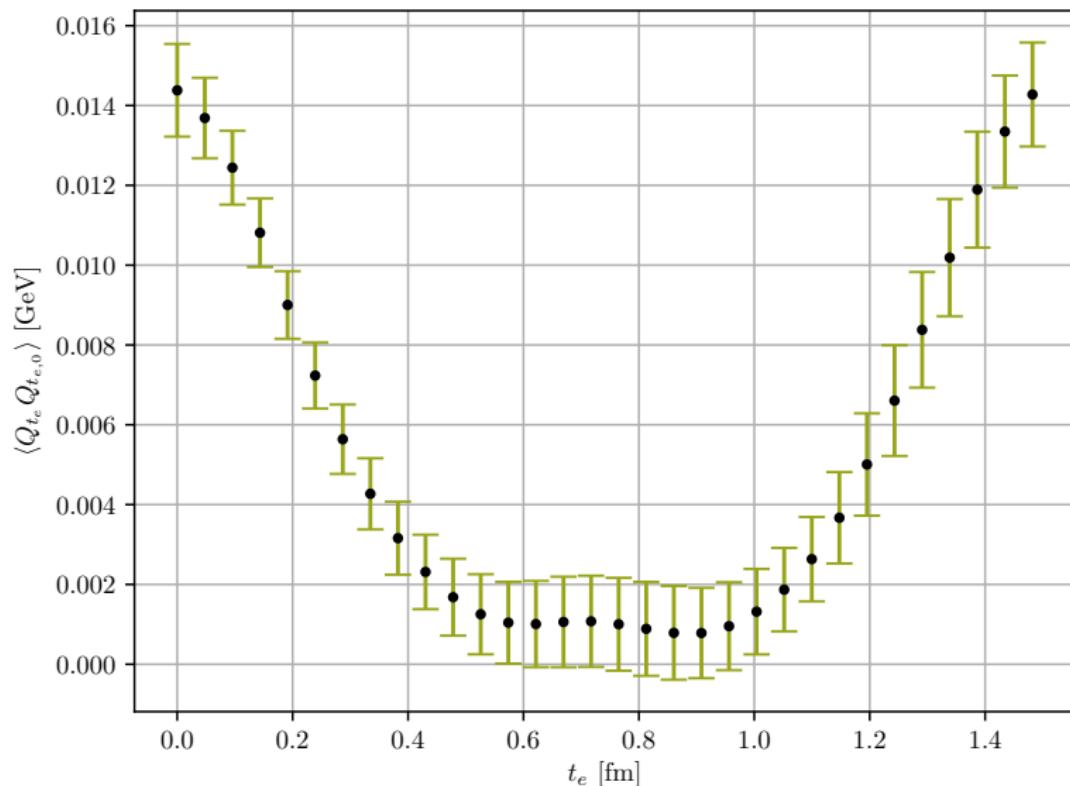
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- We since the ensembles are of different lattice sizes, we plot th D_1 separately.

The topological charge correlator



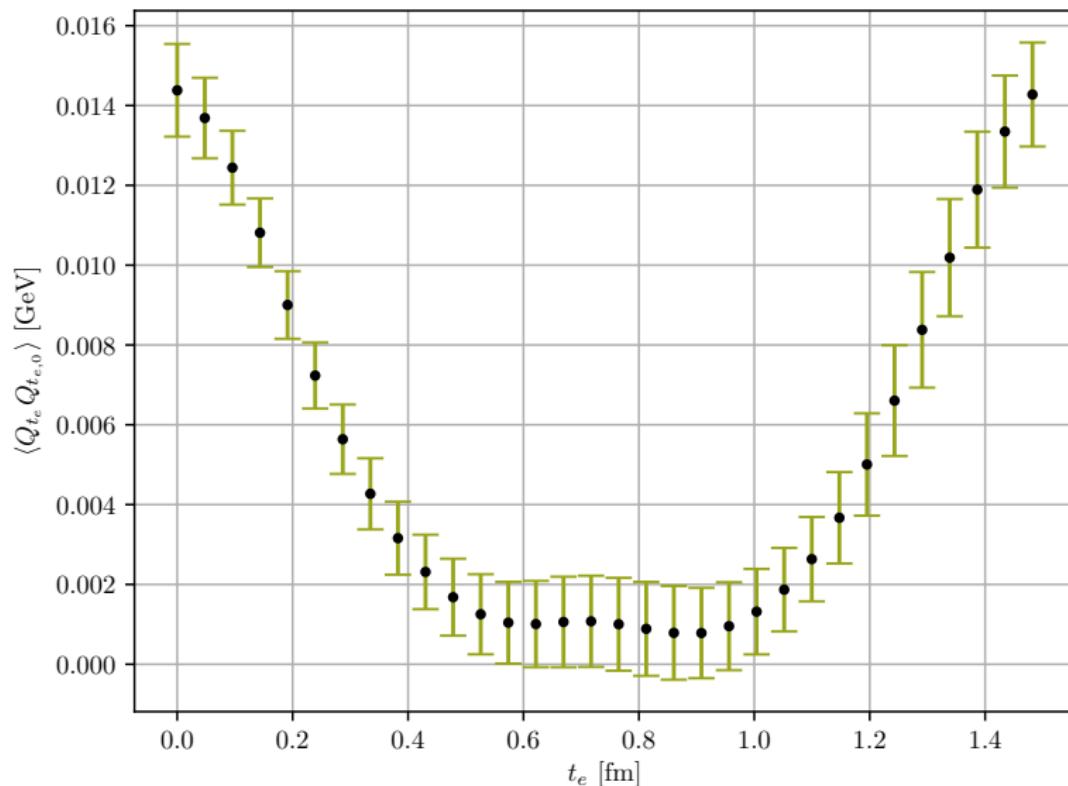
- The topological charge correlator for all of the ensembles except D_1 . The x -axis contains the sink-source separation, as the source $q(0)$ is placed at $t_e = 0$ fm, and the sink $q(t_e)$ is taken at t_e .
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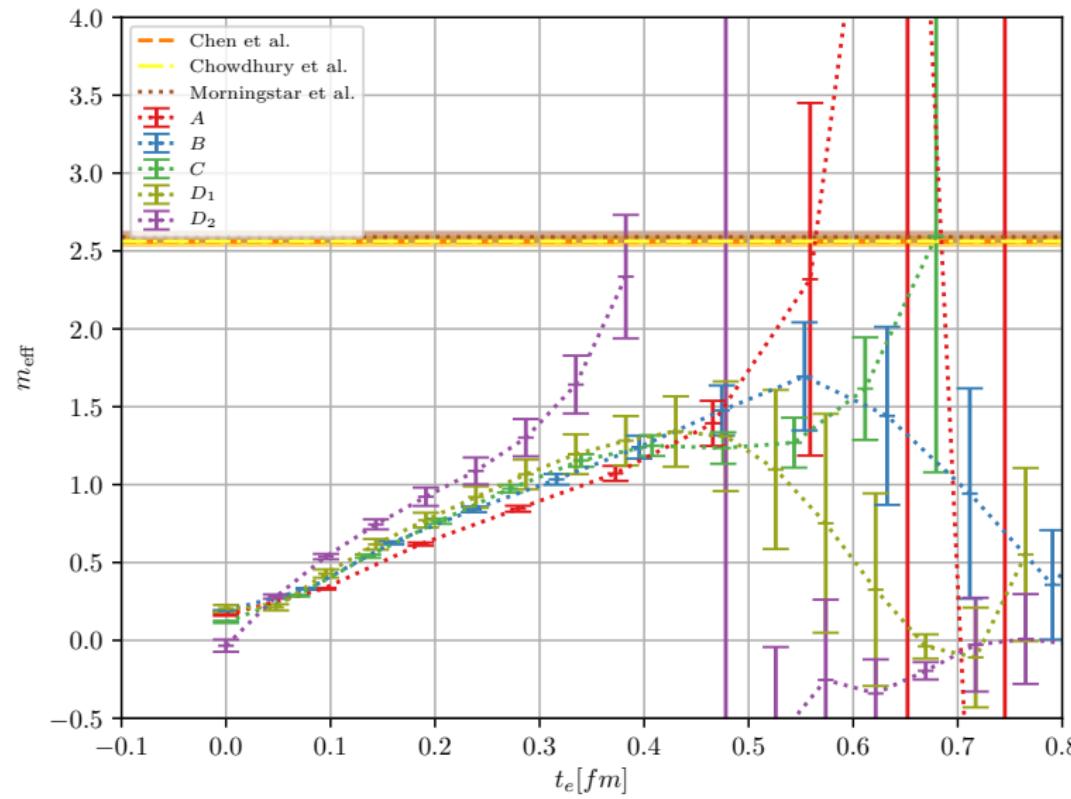
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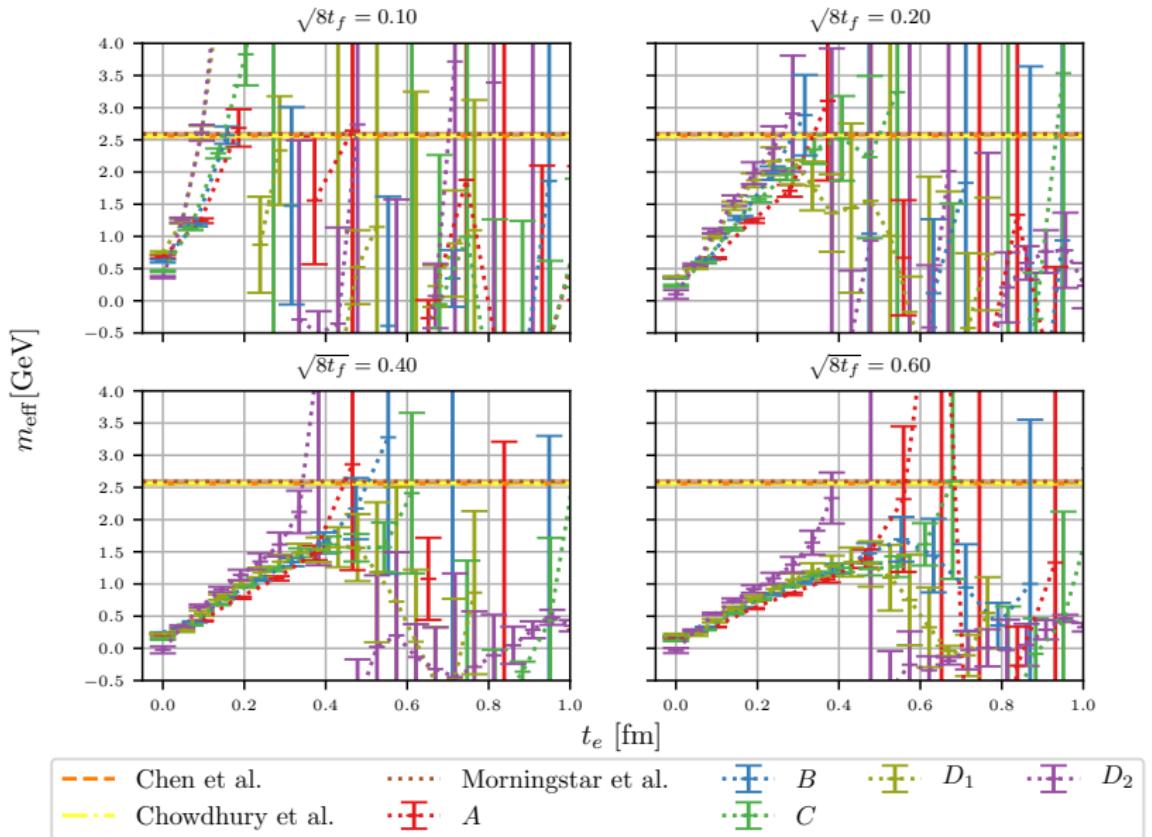
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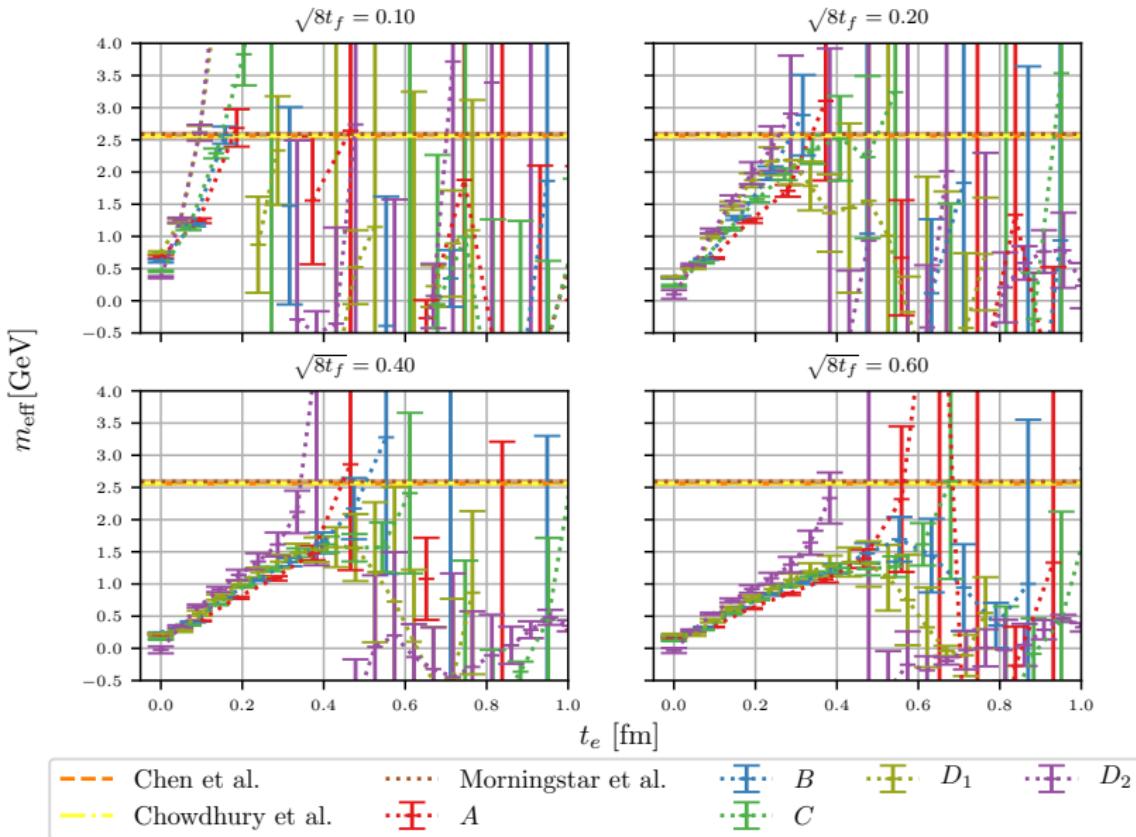


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Conclusion, future developments
and final thoughts

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Questions?

References

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- [4] Hans Munthe-Kaas. Runge–Kutta methods on Lie groups. *BIT Numerical Mathematics*, 38(1):92–111, March 1998. ISSN 0006-3835, 1572-9125. doi: 10.1007/BF02510919. URL <http://link.springer.com/10.1007/BF02510919>.

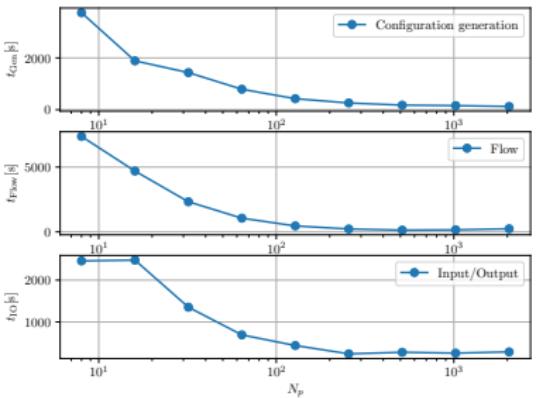
Extras

Scaling

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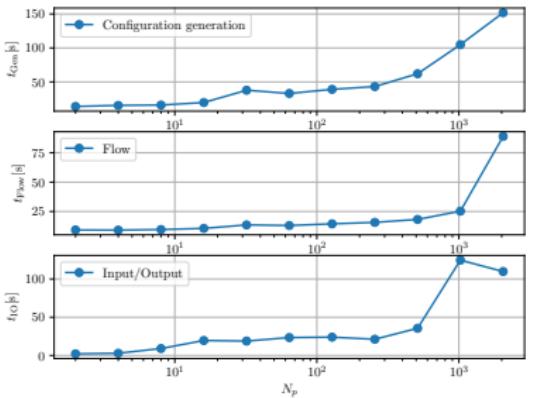


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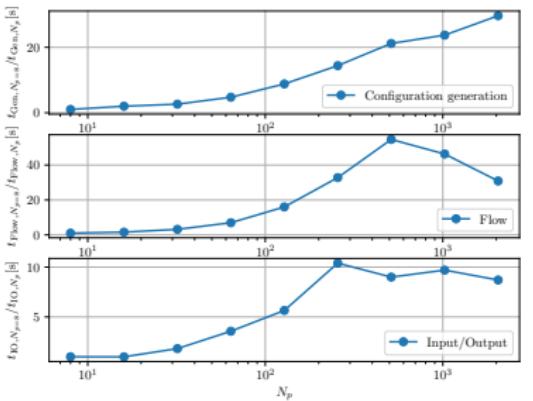
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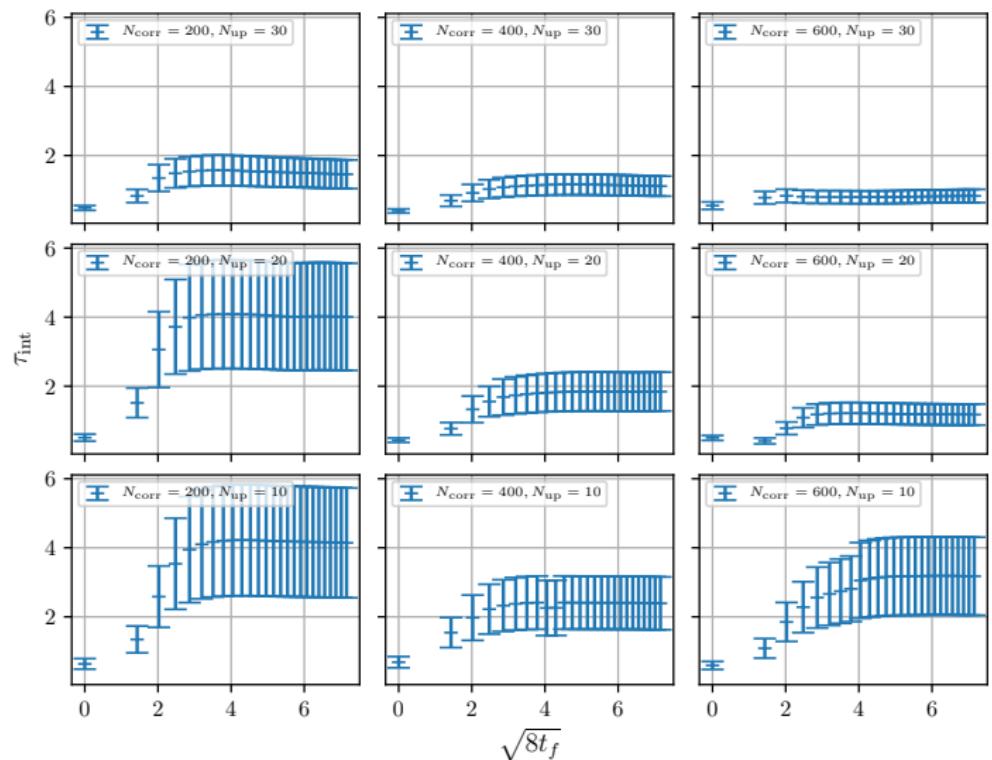
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Optimizing the gauge configuration generation

- 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 $\sqrt{8t_f}$.

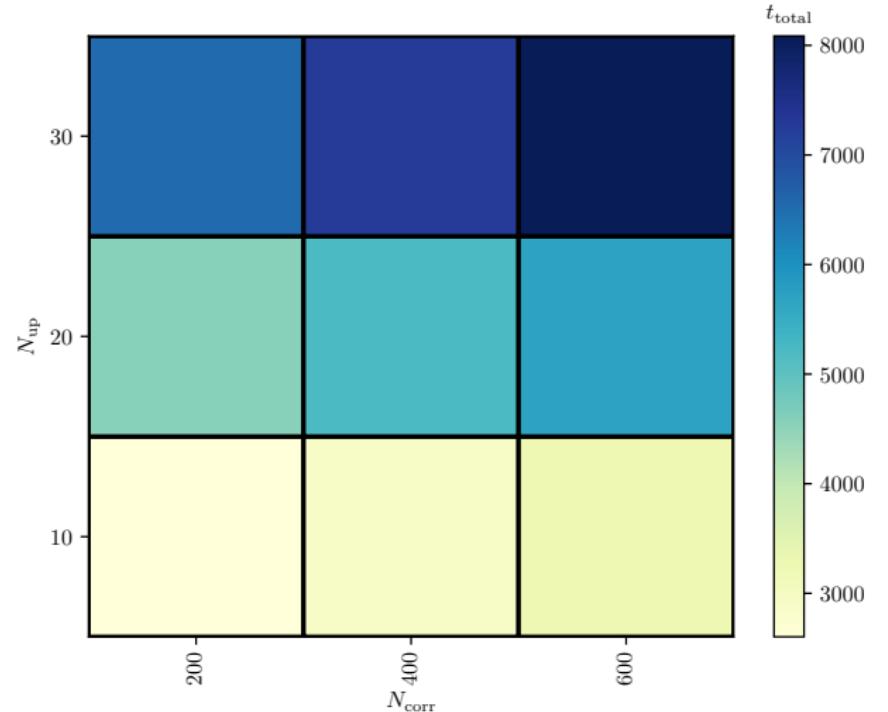
Generated 200 configurations for a lattice of size $N^3 \times N_T = 16^3 \times 32$ and $\beta = 6.0$, for combinations of $N_{\text{corr}} \in [200, 400, 600]$ and $N_{\text{up}} \in [10, 20, 30]$.

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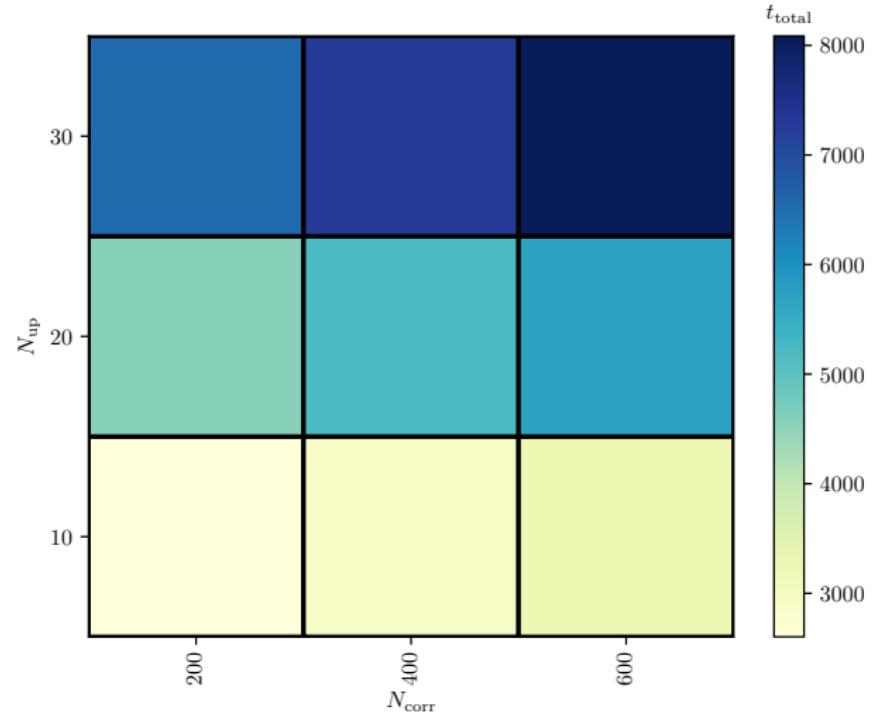
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- **Validation testing.** Cross checking results with a configuration from Chroma.

Additional ensembles

- Additional ensembles made in order to illuminate additional aspects of the topological charge.
- Supporting ensembles made on Smaug. All ensembles were flown $N_{\text{flow}} = 1000$ steps with $\epsilon_{\text{flow}} = 0.01$.

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)

Verifying the integration

- The values we will test the integrator against.

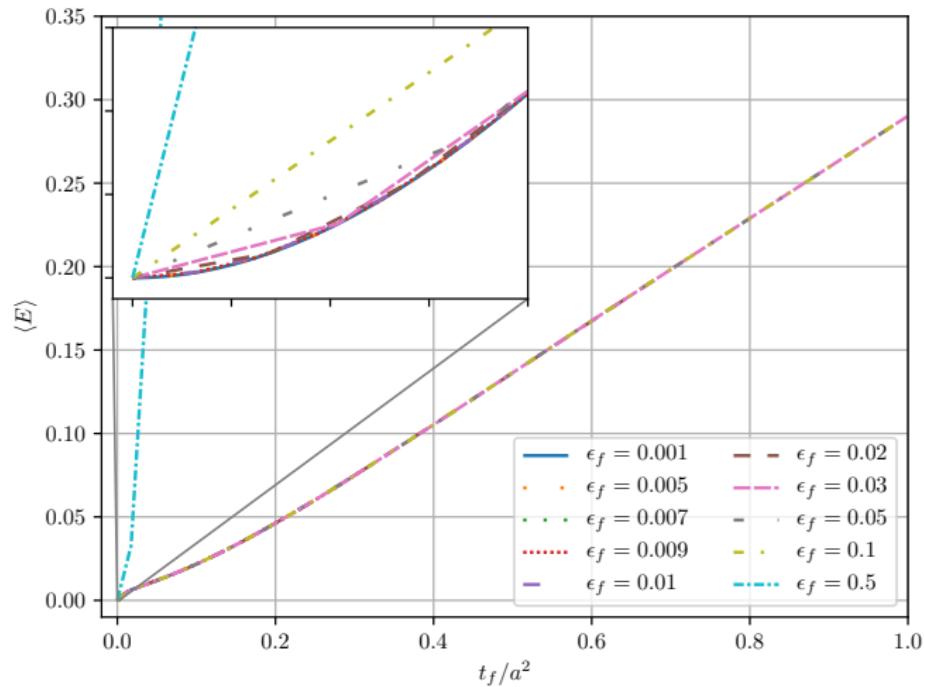
Testing the integrator for different integration steps ϵ_f .

ϵ_f	0.001	0.005	0.007	0.009	0.01	0.02	0.03	0.05	0.1	0.5
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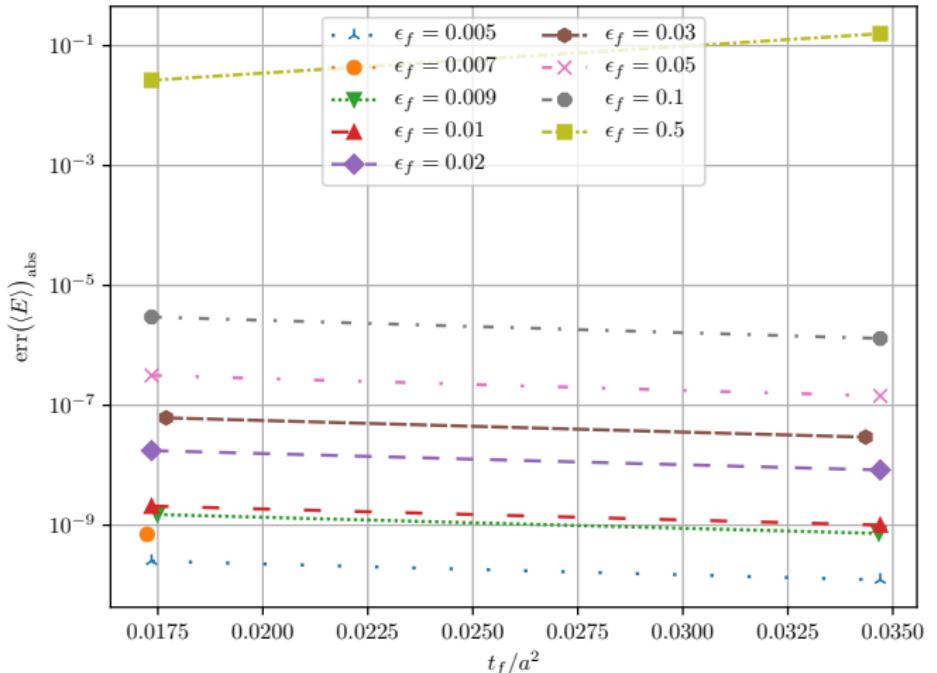
Lattice size $N^3 \times N_T = 24^3 \times 48$ with $\beta = 6.0$.

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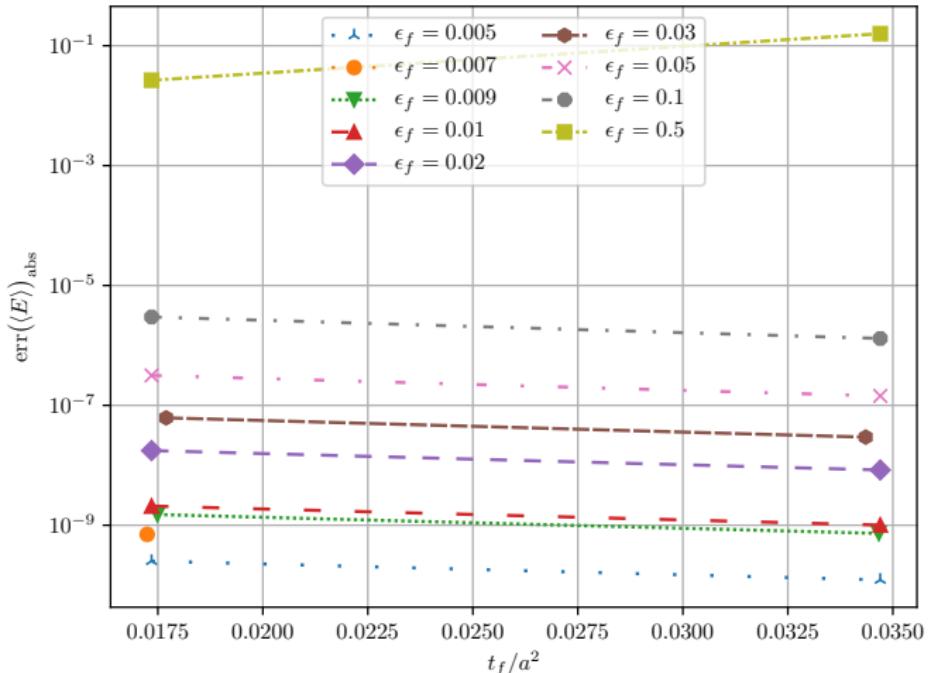
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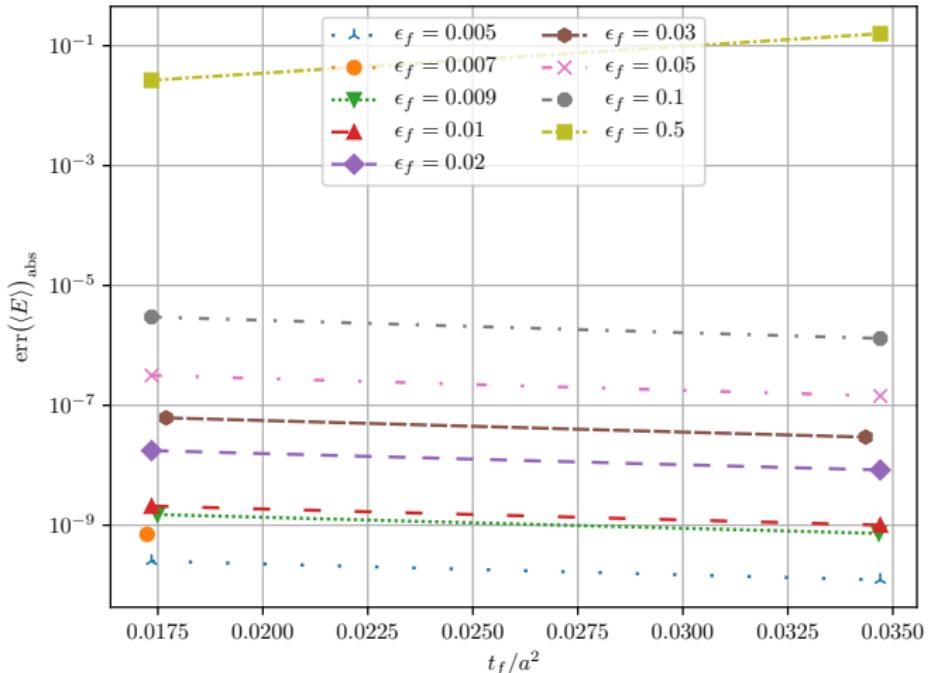
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