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

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Introduction

- Quantum Chromodynamics(QCD).

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- **GLAC.** Will briefly present the code which we developed as well as some benchmarks. We will also present the Metropolis algorithm.
- **Results.** We will present the results obtained from pure gauge calculations.

Structure

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- Lattice QCD.
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Quantum Chromodynamics(QCD)

- The standard model: Six quarks and eight gluons

2

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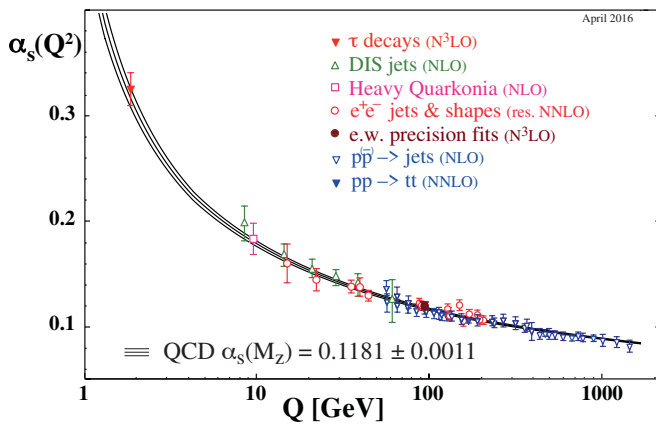- Highly nonlinear due to gluon self-interactions

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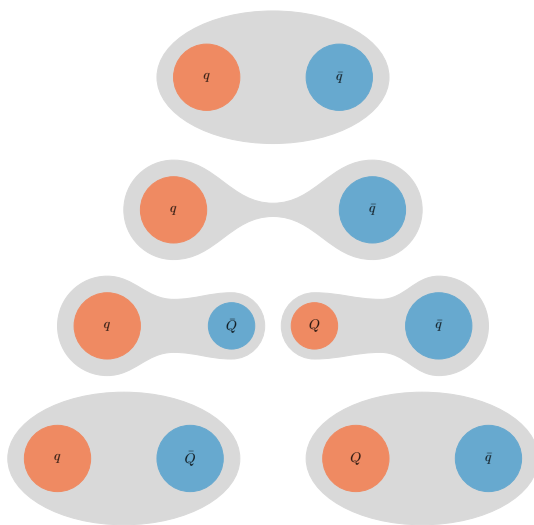- Highly nonlinear due to gluon self-interactions
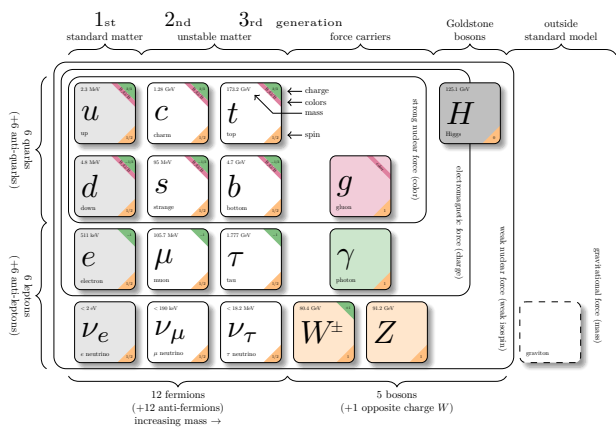
Consists of the innermost square of the six quarks and the gluons.

- 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.**
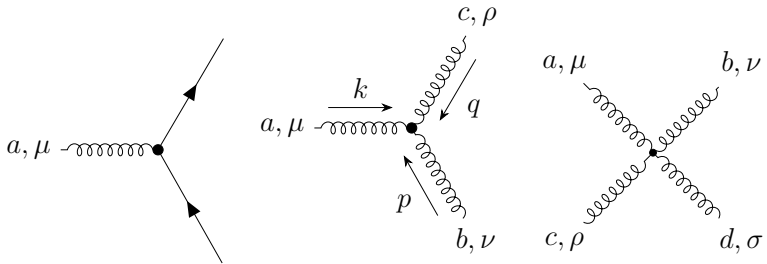
The QCD Lagrangian

$$\mathcal{L}_{\text{QCD}} = \sum_{f=1}^{N_f} \bar{\psi}^{(f)} \left(i\slashed{D} - m^{(f)} \right) \psi^{(f)} - \frac{1}{4} G^a_{\mu\nu} G^{a\mu\nu},$$

with action

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

Topology in QCD

- Instantons

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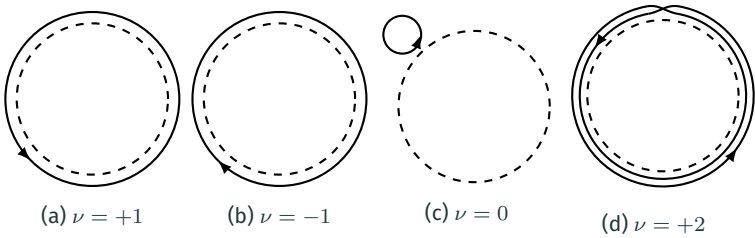(a) $\nu = +1$ (b) $\nu = -1$ (c) $\nu = 0$ (d) $\nu = +2$

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

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- 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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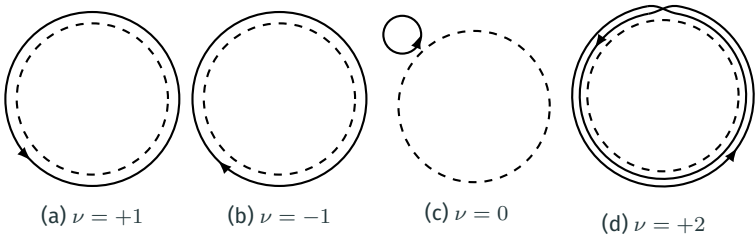- Topological charge, Q
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A formula connecting pure gauge theory and full QCD.

$$m_{\eta'}^2 = \frac{2N_f}{f_\pi^2}\chi_{\text{top}} \tag{2}$$

- 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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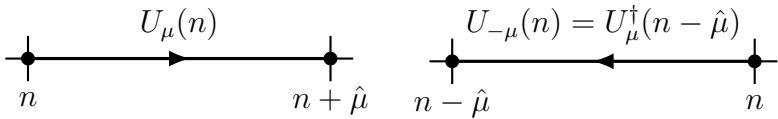
1. Divide spacetime into a cube of size $N^3 \times N_T$.
2. Fermions live on the each *point* in the cube.
3. The gauge fields live on the sites *in between* the points, and is called links.

Links

A link

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

connects one lattice site to another and is a $SU(3)$ 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

$$U_\mu(n) \rightarrow U'_\mu(n) = \Omega(n) \, U_\mu(n)\Omega(n + \hat{\mu})^\dagger,$$
$$U_{-\mu}(n) \rightarrow U'_{-\mu}(n) = \Omega(n) \, U_\mu(n - \hat{\mu})^\dagger\Omega(n - \hat{\mu})^\dagger.$$

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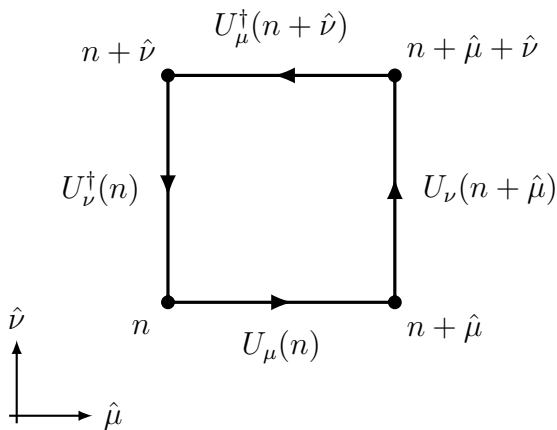$$U_{-\mu}(n) \to U'_{-\mu}(n) = \Omega(n)\, U_\mu(n - \hat{\mu})^\dagger\Omega(n - \hat{\mu})^\dagger.$$

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,

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

The Wilson gauge action is given as

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

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

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- 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 $SU(3)$ Yang-Mills theory on the lattice

A lattice configuration consists of $SU(3)$ matrices,

- The $SU(3)$ 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.

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

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

14

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

with

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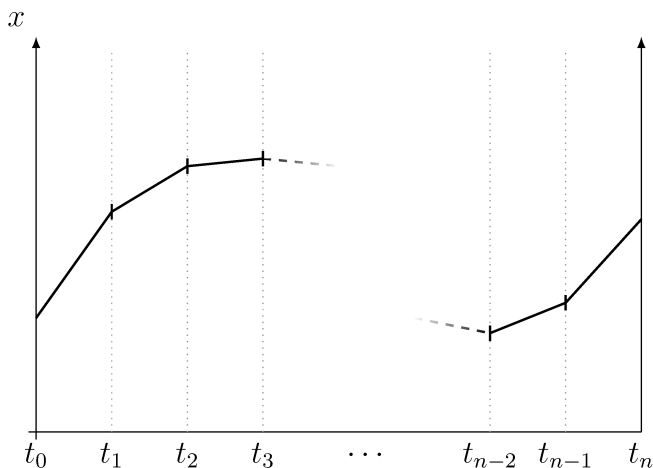
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$$Z = \int \mathcal{D}U e^{-S_G[U]}.$$

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.

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...

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- We perform an average of the created configurations.

The Metropolis algorithm

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.

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

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.
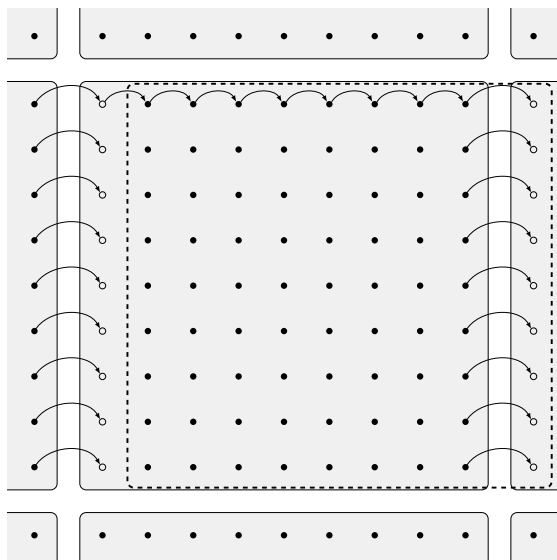
- An illustration of the lattice shift.
- The links U_ν of the lattice are copied over to a temporary lattice shifted in direction $\hat{\mu}$.
- The face that is shifted over to an adjacent sub-lattice is shared through a non-blocking MPI call, while we copy the links to the temporary lattice.
- Allows 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*
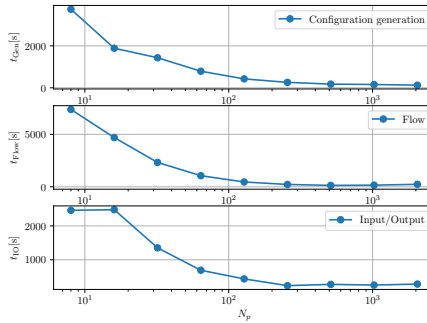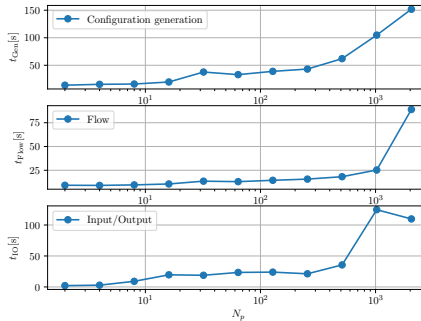
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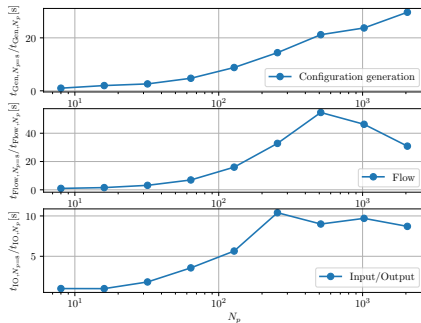- **Weak scaling:** *fixed problem per processor* and a *variable N_p cores*.
- **Speedup:** defined as $S(p) = \frac{t_{N_p,0}}{t_{N_p}}$.

- 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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Optimizing the gauge configuration generation

Generated 200 configurations for a lattice of size $N^3 \times N_T = 16^3 \times 32$ and $\beta = 6.0$.
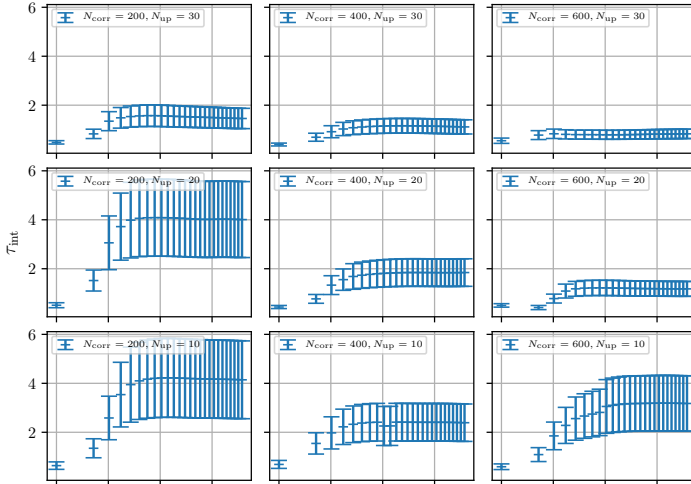
- We run for different values for N_{up} and N_{corr} to see what gives optimizes **computational cost** and **autocorrelation**.

- 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 $N_{\mathrm{corr}} \in [200, 400, 600]$ and $N_{\mathrm{up}} \in [10, 20, 30]$, plotted against flow time $\sqrt{8t_f}$.

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

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Gradient flow

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

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

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

$$G_{\mu\nu}(x, t_f) = \partial_\mu B_\nu(x, t_f) - \partial_\nu B_\mu(x, t_f) - i[B_\mu(x, t_f), B_\nu(x, t_f)], \tag{6}$$
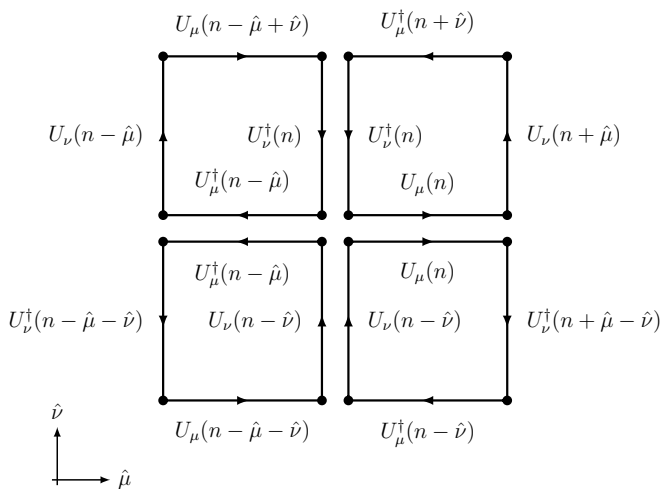
with the initial condition of eq. (4) being the fundamental gauge field,

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

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

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Results

The clover field strength definition

· We will use the clover field strength definition in gauge observables

Energy definition

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

- We can use this definition to set a scale.

Scale setting

Topological charge definition

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

with the charge density given by

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

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- 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 susceptibility

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.