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INVESTIGATION OF THE COLUMBIA PLOT IN THE HIGH MASS REGION

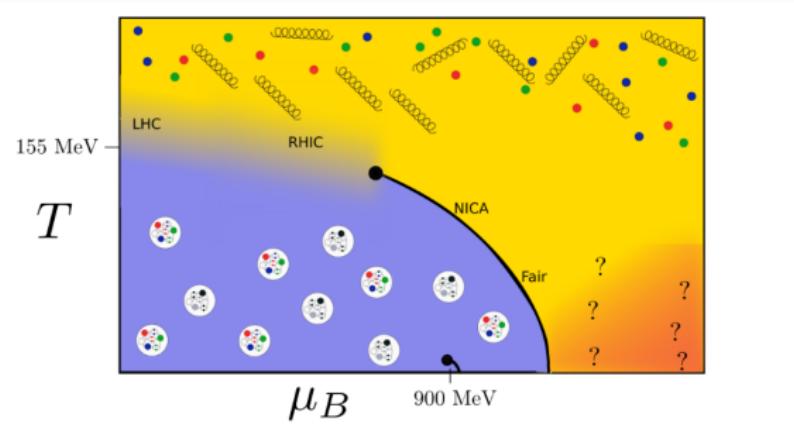
Marc-André Petri in collaboration with S. Borsanyi, J. Guenther and
R. Kara

Strong-HFFF Workshop - Sicily 2023

29. September 2023

Bergische Universität Wuppertal

QCD Phase-Diagram



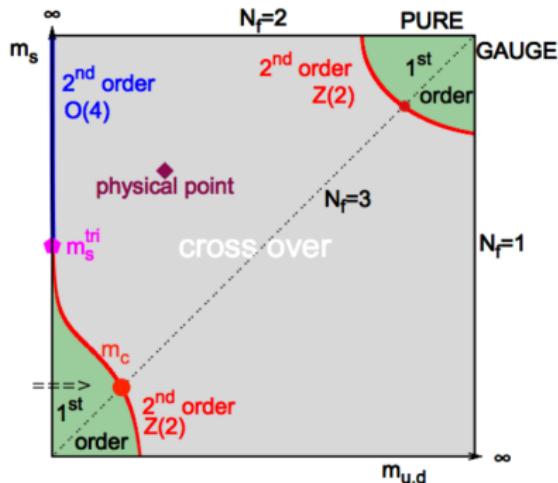
Guenther arxiv:2201.02072

- $\mu = 0 \rightarrow$ Crossover determined by theory and experiment
- $\mu > 0$ Hard to investigate with lattice QCD due to a sign problem

Columbia Plot

Columbia Plot for 0
chemical potential

- Physical masses
 \Rightarrow Crossover
(*Fodor et. al.*
0611014)
- Pure gauge theory:
Latent heat in cont.
limit determined by
Borsanyi et. al.
2202.05234
 \Rightarrow 1st order



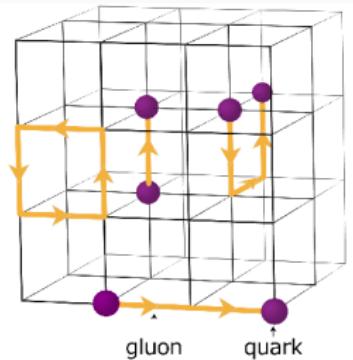
One of three possible Columbia Plots
Forcrand et. al. arxiv:1702.00330

Details on lower left: see talk
Julian Bernhardt

Challenges when Investigating Phase Transitions on the Lattice

- 1st order phase transition has super critical slowing down
 - Both phases have to be sampled for investigations of the phase transition
- 2nd order phase transition has critical slowing down
 - Large autocorrelation of simulated data.
- Simulating with fermions has high computational cost (scales inverse with the mass of the fermions)
 - Problem of generating enough statistics or independent samples

Introduction to Lattice QCD



Sketch of a lattice

Lattice QCD

- Discretize the spacetime with spacing a
- Place Spinors ψ at lattice points
- Place Gauge Field as links U_μ in between
- Choose suitable action for Gauge field i.e $S_G[U] = -\frac{\beta}{3} \sum_{n \in \Lambda} \sum_{\mu < \nu} \Re \text{tr}(\mathbb{1} - P_{\mu\nu}(n))$

Suitable Observables for Investigation

- Polyakov Loop and its susceptibility:

$$P = \frac{1}{N_s^3} \sum_{\vec{x}} P_{\vec{x}} = \frac{1}{N_s^3} \sum_{\vec{x}} \text{tr} \left[\prod_{\tau} U_0(\vec{x}, \tau) \right] \quad (1)$$

$$\chi = N_s^3 (\langle |P|^2 \rangle - \langle |P| \rangle^2) \quad (2)$$

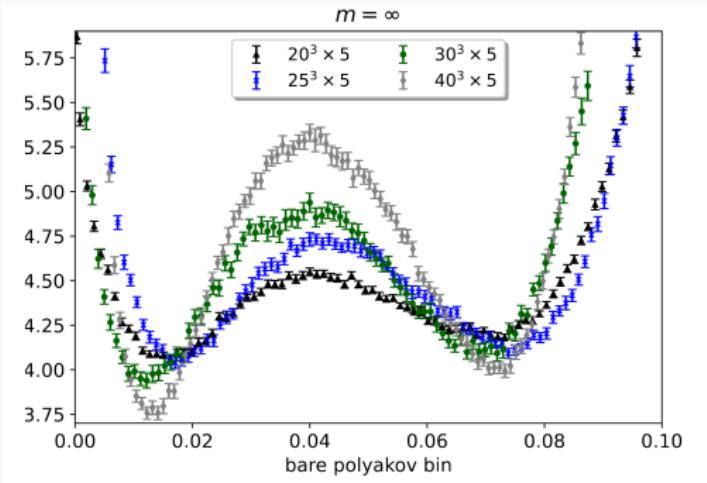
- Third-order Binder cumulant of the Polyakov loop:

$$b_3 = \frac{\langle |P|^3 \rangle - 3\langle |P| \rangle \langle |P|^2 \rangle + 2\langle |P| \rangle^3}{(\langle |P|^2 \rangle - \langle |P|^2 \rangle)^{\frac{3}{2}}} \quad (3)$$

- Latent heat:

$$\Delta \left(\frac{\epsilon - 3p}{T^4} \right) = N_t^4 a \frac{\partial \beta}{\partial a} [S_{\text{hot}} - S_{\text{cold}}] \quad (4)$$

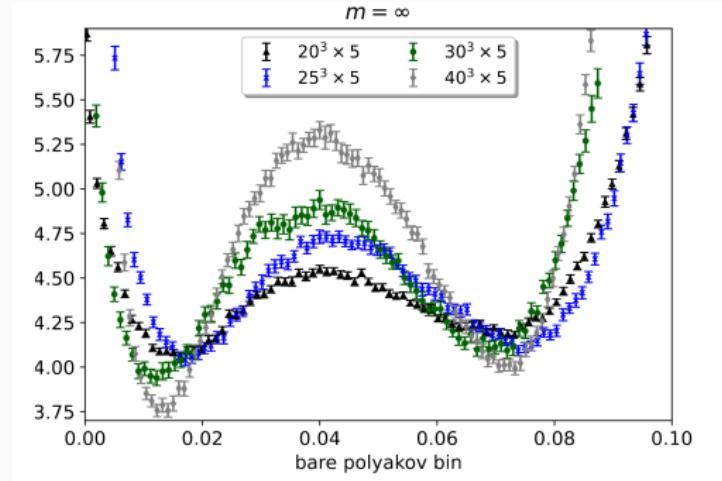
Super critical slowing down – Quenched QCD



Wuppertal-Budapest arxiv: 2212.10155

- Problem: The system is more likely to freeze in one of the two phases

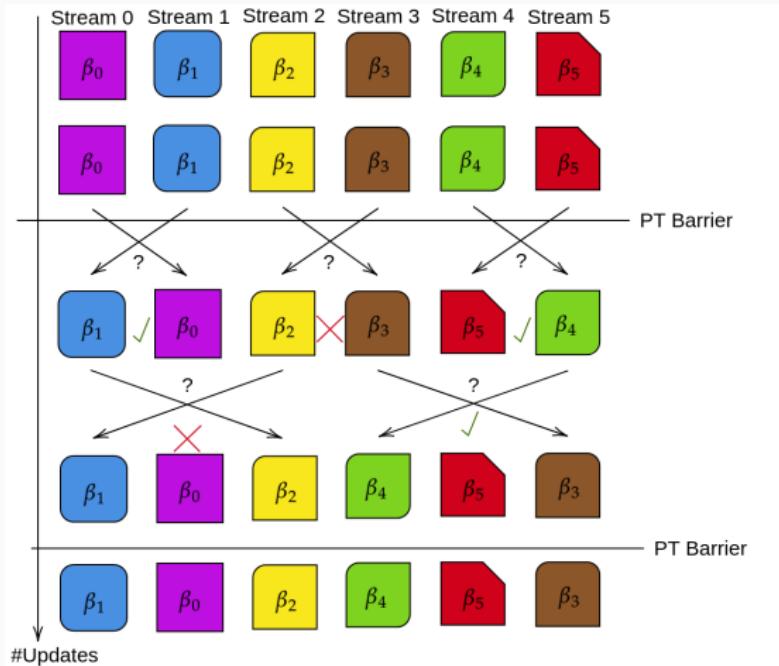
Super critical slowing down – Quenched QCD



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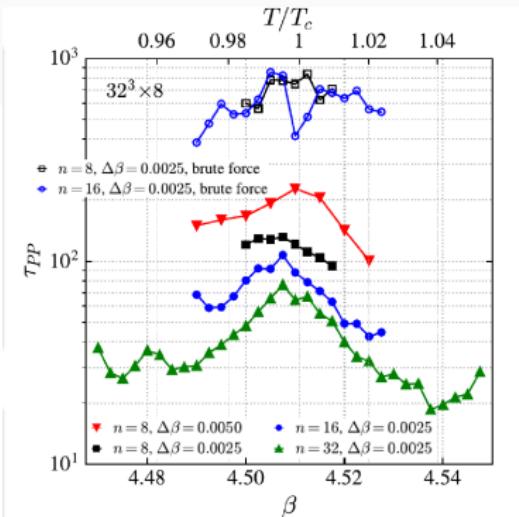
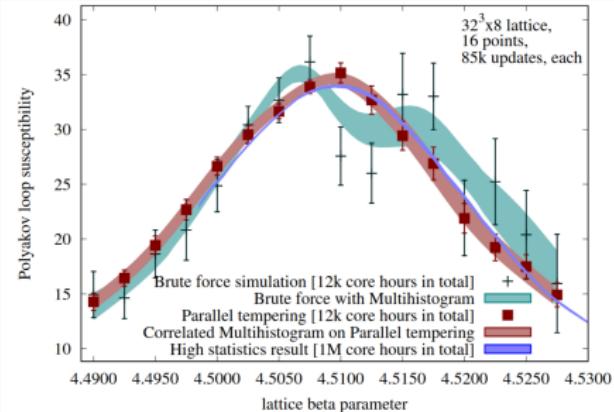
- Problem: The system is more likely to freeze in one of the two phases
- → One Ansatz: Parallel Tempering (*arxiv: 9205018 ,9810032*)
Marc-André Petri (Bergische Universität Wuppertal)

Parallel Tempering - Principle



Principle of the Parallel Tempering Algorithm. β indicates inverse Temperature

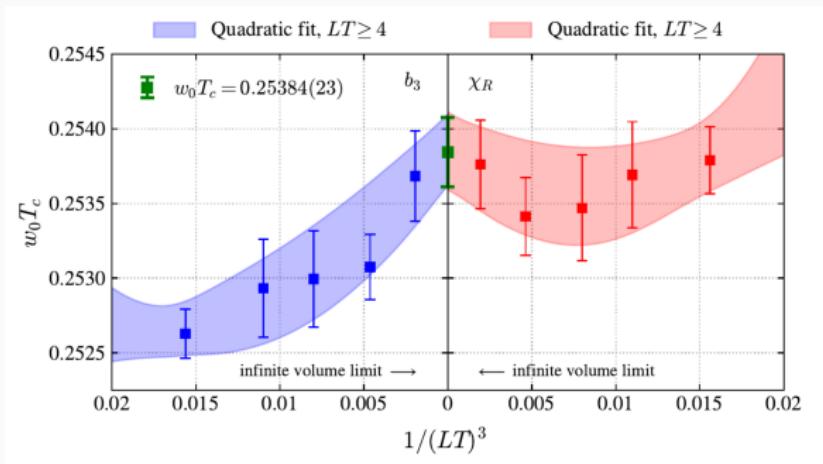
Parallel Tempering – Consequences in Quenched QCD



Wupperta-Budapest arxiv: 2202.05234

- Autocorrelation time drops significantly
→ More precise simulations with the same effort

Determine Transition Temperature and Latent Heat



Wuppertal-Budapest arxiv: 2202.05234

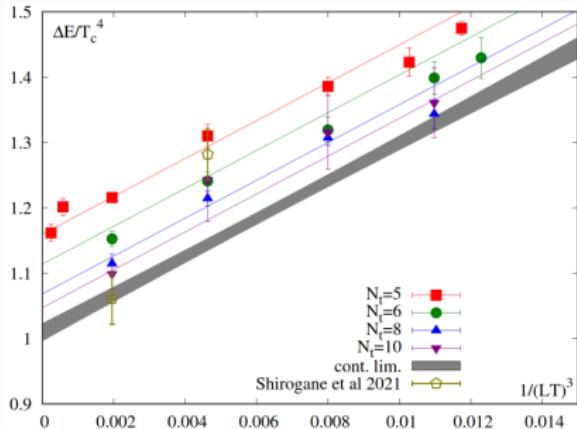
Determined transition temperature (in lattice units):

$$w_0 T_c = 0.25384(11)_{\text{stat}}(21)_{\text{sys}}$$

First per-mil accurate result in QCD thermodynamics

Marc-André Petri (Bergische Universität Wuppertal)

Determine Transition Temperature and Latent Heat



Wuppertal-Budapest arxiv: 2202.05234

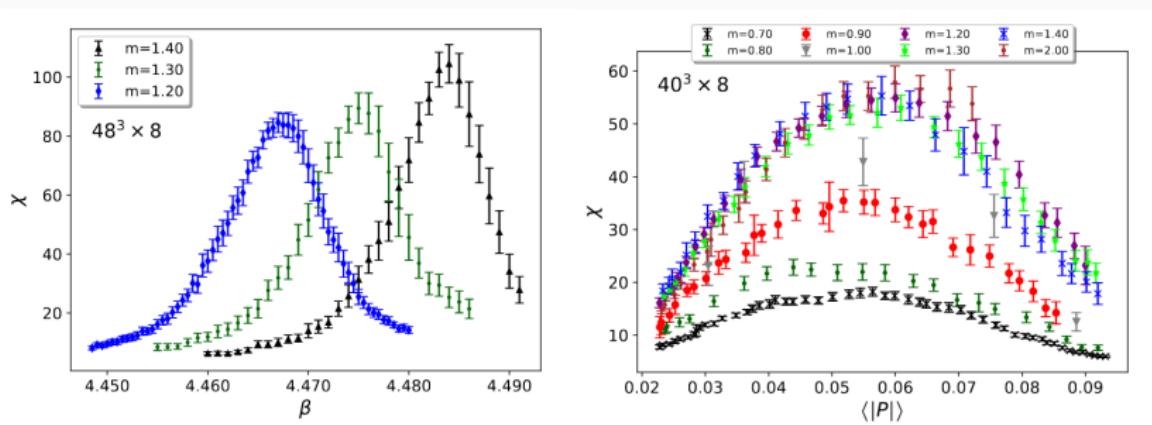
- Determined latent heat

$$\Delta\left(\frac{\epsilon - 3p}{T^4}\right) = 1.025(21)_{\text{stat}}(27)_{\text{sys}} \quad (5)$$

→ Confirms first order phase transition

Parallel Tempering applied to Dynamical QCD

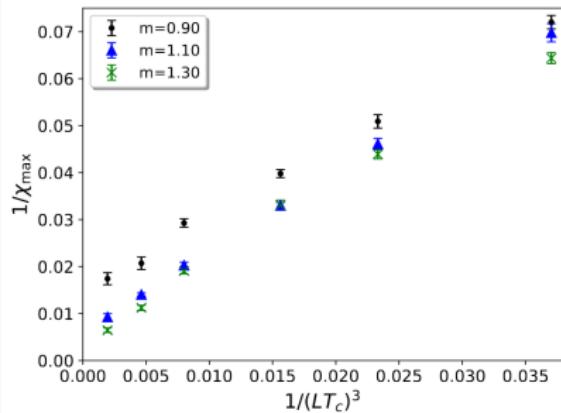
Now include dynamical quarks with large but finite mass and measure peak position again for different masses



Wuppertal-Budapest arxiv: 2212.04192

Determine peak position for each mass and volume simulated

Parallel Tempering applied to Dynamical QCD

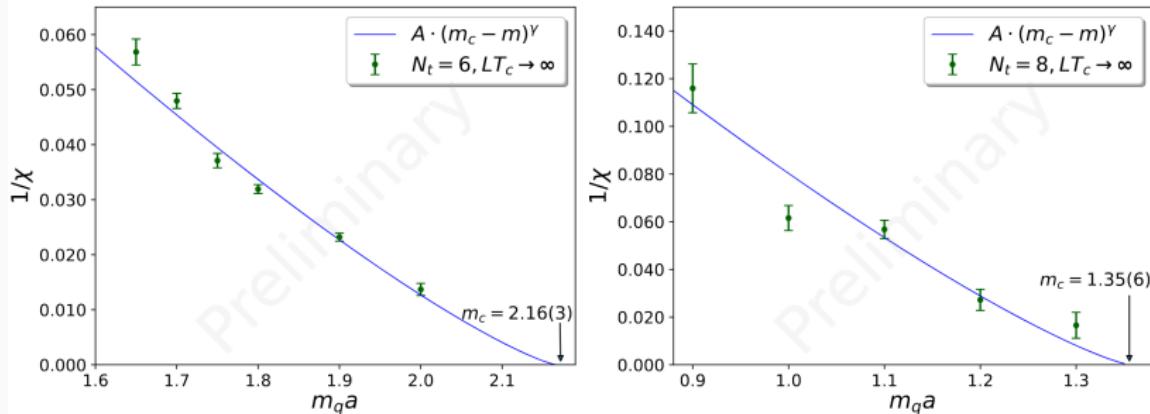


Wuppertal-Budapest 2212.04192

Fit functions

- Linear: $\chi^{-1}(LT_c) = a + b \left(\frac{1}{LT_c^3} \right)$
- With "effective exponent": $\chi^{-1}(LT_c) = a + b \left(\frac{1}{LT_c^3} \right)^c$

Determine m_c



R. Kara Lattice 2022

Note: No continuum limit of the critical mass possible yet, due to critical slowing down and additional computational costs in including fermions into the simulation.

Improvement but not the solution

- Autocorrelation time was decreased significantly
 - Transition temperature on per mil accuracy was determined
 - Latent Heat > 0 was determined proving the 1st order phase-transition
 - **But:** If one reduces the mass of fermions (uses Dynamical Fermions) the problem of adding fermions also add up to the already existing (super) critical slowing down
- We could try new kinds of algorithms in the high mass region or in the pure gauge theory.

Procedure of testing new algorithms for Gauge theories

- Work in an easier gauge group $SU(2)$:
 1. System gives far easier environment to test into
 2. Simulations take less time than $SU(3)$ simulations
 3. System is in the same universality class (scaling behavior) as the 3D Ising modell (very simple)
- If algorithms don't work in $SU(2)$ they should not work in $SU(3)$ either
- If algorithms work in $SU(2)$ they might as well be applicable for $SU(3)$

Cluster Algorithm for Gauge theories?

- Idea: build Clusters, that flip the sign of the trace of the Polyakov Loop

Why could something like that work?

- $SU(2)$ and the 3D Ising model are in the same Universality class → $SU(2)$ can be mapped into the Ising Model
- For the Ising Model such Algorithms are well known to solve problem of critical slowing down
(Wolff DOI: 10.1103/PhysRevLett.62.361 ,
Swendsen-Wang, DOI: 10.1103/PhysRevLett.58.86)

How is SU(2) mapped into the Ising Model?

- Action of SU(2)

$$S = -\frac{\beta}{2} \sum_{P_{\mu,\nu}} \text{Tr} P_{\mu,\nu}$$

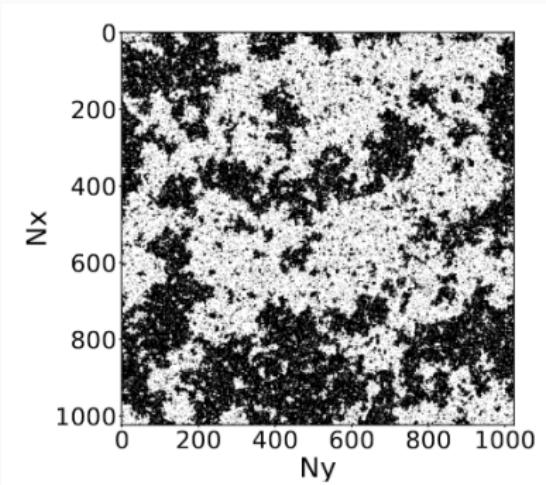
- Hamiltonian of the Ising Model

$$H = -\frac{1}{2} \sum_{\langle ij \rangle} s_i s_j k_{ij}$$

- Idea for connecting them

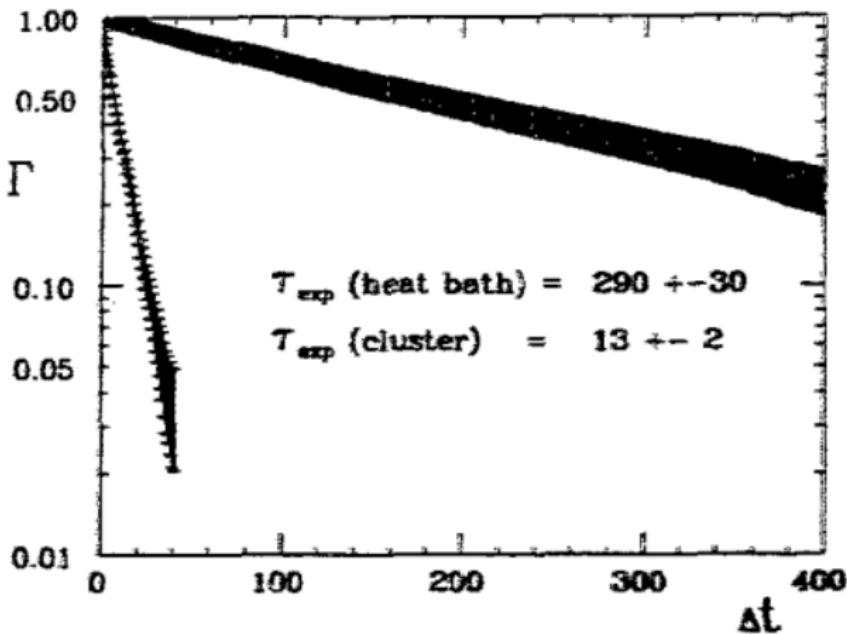
$$s_i = \text{sgn}(\text{Tr}(U_i))$$

$$\Rightarrow k_{ij} = \frac{\text{Tr} P}{\text{sgn} \text{Tr} U_i \text{sgn} \text{Tr} U_j}$$



2D Ising Model near the Critical point

Can this work?



Evertz et. al DOI: 10.1016/0920-5632(91)90886-J

Conclusion

- Algorithmic ideas or mixing of algorithms can help with sampling more efficiently (Parallel Tempering)
- Cluster algorithms which work very good for Spin systems (eg. 3D Ising Model) should be able be implemented in a similar way for gauge theories ($SU(2)$ maybe also $SU(3)$) due to the fact that they are in the same universality class (not clear for $SU(3)$)
- Mapping of $SU(2)$ into an Ising Model in test stage at the moment

Problems and ideas to solve for upper right corner

Still existing Problems

- (Super) critical slowing down in the 1st and 2nd order
(partially improved by using parallel tempering algorithm)
- Computational costs of including dynamical fermions → No continuum limit for m_c in upper right corner due to the upper point

Possible Solutions

- Global heatbath update
- Exploiting of expansions of fermion formulations similar to
arxiv: 1805.03560

Thank you for your attention!
Any Questions?

Backup - Introduction to lattice QCD SU(3)

In the continuum we have the action for the Gluons:

$$S_G[A] = \frac{1}{4g^2} \sum_{i=1}^8 \int d^4x F_{\mu\nu}^{(i)}(x) F_{\mu\nu}^{(i)}(x) \quad (6)$$

and the fermions:

$$S_F[\psi, \bar{\psi}, A] = \sum_{f=1}^{N_F} \int d^4x \bar{\psi}^{(f)}(x) (\gamma_\mu (\partial_\mu + iA_\mu) + m^{(f)}) \psi^{(f)}(x) \quad (7)$$

Backup - Introduction to lattice QCD SU(3)

Plaquette (smallest simply connected loop on the lattice)

$$P_{\mu\nu}(n) = U_\mu(n)U_\nu(n + \hat{\mu})U_\mu^\dagger(n + \hat{\nu})U_\nu^\dagger(n). \quad (8)$$

Wilson gauge is one action that approaches the continuum version for $a \rightarrow 0$:

$$S_G[U] = -\frac{\beta}{3} \sum_{n \in \Lambda} \sum_{\mu < \nu} \Re \text{tr}(\mathbb{1} - P_{\mu\nu}(n)) \quad (9)$$

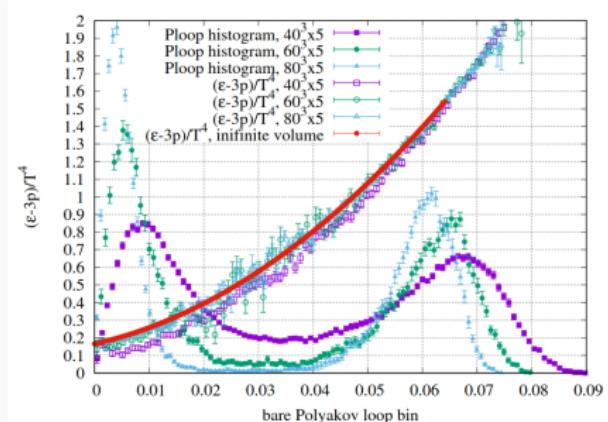
Gauge variables $U_\mu(n)$ introduced to make naive fermion action invariant under local gauge transformation and live on the links between two lattice points

$$U_\mu(n) = \exp\{iaA_\mu(n)\}$$

- Use Markov chain Monte-Carlo Algorithms to update the discretized field
- To update the gauge field one uses local update algorithms (Metropolis, Heatbath, (+Overrelaxation))
- With the including of fermions has has to use other algorithms (Hybrid Monte-Carlo is used)

→ After a certain number of updates measure observables on the sampled field (e.g Energy, Magnetization, Plaquette, Polyakov-Loop)

Backup - Determine Transition Temperature and Latent Heat



Budapest-Wuppertal arxiv: 2212.10155

- Latent heat defined via the trace anomaly
- Find minimum of the Polyakov Loop histogram
→ The trace anomaly can then be evaluated in both phases

Backup - How does such a Cluster-Algorithm Work

- Let's first look at the Cluster Algorithm in the Ising Model (here Wolff as an example)

+	+	+	+	-	-	-
+	-	-	-	+	-	-
+	-	+	-	-	+	-
-	+	+	-	+	+	-
+	-	+	-	+	+	+

Sketch how the Wolff Algorithm works

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+	-	+	-	+	+	+

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+	-	+	+	+	+	-
-	+	+	-	+	+	-
+	-	+	-	+	+	+

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