

Solution of the sign problem in the Potts model at fixed baryon number

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Motivation for canonical formulation of QCD

- ▶ Consider the **grand-canonical partition function** of QCD:

$$Z_{\text{GC}}^{\text{QCD}}(\mu) = \text{Tr} [e^{-\mathcal{H}(\mu)/T}] = \text{Tr} \prod_t \mathcal{T}_t(\mu)$$

- ▶ The **sign problem** of QCD is a **manifestation of huge cancellations** between different states:

- ▶ all states are present for any μ and T
- ▶ some states need to cancel out at different μ and T

- ▶ In the **canonical formulation**:

$$Z_{\text{C}}^{\text{QCD}}(N_Q) = \text{Tr}_{N_Q} [e^{-\mathcal{H}(\mu)/T}] = \text{Tr} \prod_t \mathcal{T}_t^{(N_Q)}$$

- ▶ dimension of Fock space tremendously reduced
- ▶ less cancellations necessary
- ▶ e.g. $Z_{\text{C}}^{\text{QCD}}(N_Q) = 0$ for $N_Q \neq 0 \pmod{N_c}$

Motivation for canonical formulation of QCD

Canonical transfer matrices can be obtained explicitly!

- ▶ based on the dimensional reduction of the QCD fermion determinant [Alexandru, Wenger '10; Nagata, Nakamura '10]
- ▶ identification of transfer matrices [Steinhauer, Wenger '14]

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- ▶ **Motivation**
 - ▶ QCD in the heavy-dense limit
 - ▶ Canonical formulation
 - ▶ Absence of the sign problem at strong coupling
- ▶ **Solution in the 3-state Potts model**
 - ▶ Canonical formulation
 - ▶ Bond formulation and cluster algorithm
 - ▶ Solution of the sign problem
 - ▶ cf. [Alford, Chandrasekharan, Cox, Wiese 2001]

Dimensional reduction of QCD

- ▶ Reduced Wilson fermion determinant is given by

$$\det M_{p,a}(\mu) \propto \prod_t \det Q_t^+ \cdot \det [e^{+\mu L_t} \cdot \mathbb{I} \pm \mathcal{T}]$$

where \mathcal{T} is a product of transfer matrices given by

$$\mathcal{T} = \prod_t Q_t^+ \cdot \mathcal{U}_t \cdot (Q_{t+1}^-)^{-1}$$

with

$$Q_t^\pm = B_t P_\pm + P_\mp.$$

- ▶ Fugacity expansion yields with $N_Q^{\max} = 2 \cdot N_c \cdot L_s^3$

$$\det M_a(\mu) = \sum_{N_Q=-N_Q^{\max}}^{N_Q^{\max}} e^{\mu N_Q/T} \cdot \det M_{N_Q}$$

Heavy-dense limit of grand-canonical QCD

- ▶ The **heavy-dense approximation** in general consists of taking the limit $\kappa \equiv (2m+8)^{-1} \rightarrow 0$, $\mu \rightarrow \infty$ while keeping $\kappa e^{+\mu}$ fixed.
- ▶ Better: just drop the spatial hopping terms, but **keep forward and backward hopping in time**:
 - ▶ system of static **quarks and antiquarks**
- ▶ Reduced Wilson fermion matrix \Leftrightarrow effective action in terms of **Polyakov loops P and P^\dagger** in $d = 3$:

$$\det M_{p,a}^{HD} = \prod_{\bar{x}} \det [\mathbb{I} \pm (2\kappa e^{+\mu})^{L_t} P_{\bar{x}}]^2 \det [\mathbb{I} \pm (2\kappa e^{-\mu})^{L_t} P_{\bar{x}}^\dagger]^2$$

Heavy-dense limit of canonical QCD

- ▶ The canonical determinants are given by the trace over the minor matrix \mathcal{M} ,

$$\det M_{N_Q}^{HD} \propto \text{Tr} \mathcal{M}_{N_Q} \left[\left((2\kappa)^{+L_t} \cdot P_+ \mathcal{P} + (2\kappa)^{-L_t} \cdot P_- \mathcal{P} \right) \right]$$

where \mathcal{P} denotes the Polyakov loops $\mathcal{P}_{\bar{x},\bar{y}} = \mathbb{I}_{4 \times 4} \otimes P_{\bar{x}} \cdot \delta_{\bar{x},\bar{y}}$.

- ▶ Under $\mathbb{Z}(N_c)$ -transformation by $z_k = e^{2\pi i \cdot k / N_c} \in \mathbb{Z}(N_c)$:

$$\det M_{N_Q}^{HD} \rightarrow \det M_{N_Q}'^{HD} = z_k^{-N_Q} \cdot \det M_{N_Q}^{HD}$$

and summing over z_k yields $\det \mathcal{M}_{N_Q} = 0$ for $N_Q \neq 0 \bmod N_c$

- ▶ reduces cancellations by factor of N_c

Heavy-dense limit of canonical QCD

- ▶ Canonical determinant describing **no quarks** w.r.t. N_Q^{\max} :

$$\det M_{N_Q^{\max}}^{HD} = 1 \quad \Leftrightarrow \quad \text{quenched case}$$

- ▶ Canonical determinant describing a **single quark**, i.e. $N_Q = 1$:

$$\det M_{N_Q^{\max}-1}^{HD} = \left((2\kappa)^{L_t} + (2\kappa)^{-L_t} \right) \cdot \sum_{\bar{x}} \text{Tr } P_{\bar{x}}$$

- ▶ For **$N_Q = 2$ quarks**:

$$\begin{aligned} \det M_{N_Q^{\max}-2}^{HD} / \Omega &\propto 2 \sum_{\bar{x}} \text{Tr } P_{\bar{x}} \sum_{\bar{y}} \text{Tr } P_{\bar{y}} \\ &+ \left(4 \sum_{\bar{x}} \text{Tr } P_{\bar{x}} \sum_{\bar{y}} \text{Tr } P_{\bar{y}} - 3 \sum_{\bar{x}} (\text{Tr } P_{\bar{x}})^2 + 2 \text{Tr } P_{\bar{x}}^\dagger \right) \end{aligned}$$

- ▶ Both determinants **vanish under global $\mathbb{Z}(3)$ -transformations**.

Heavy-dense limit of canonical QCD

- ▶ Canonical determinant for $N_Q = 3$ quarks:

$$\det M_{N_Q^{\max}=3}^{HD}/\Omega = h_3 \cdot \left(4 \sum_{\bar{x}} \text{Tr} P_{\bar{x}}^\dagger \sum_{\bar{y}} \text{Tr} P_{\bar{y}} - 3 \sum_{\bar{x}} \text{Tr} P_{\bar{x}} \text{Tr} P_{\bar{x}}^\dagger + 2L_s^3 \right) \\ + h_1 \left(4 \sum_{\bar{x}} \text{Tr} P_{\bar{x}}^\dagger \sum_{\bar{y}} \text{Tr} P_{\bar{y}} + 2 \sum_{\bar{x}} (\text{Tr} P_{\bar{x}})^2 \sum_{\bar{y}} \text{Tr} P_{\bar{y}} \right. \\ \left. + 4 \sum_{\bar{x}} \text{Tr} P_{\bar{x}} \sum_{\bar{y} \neq \bar{x}} \text{Tr} P_{\bar{y}} \sum_{\bar{z}} \text{Tr} P_{\bar{z}} \right)$$

- ▶ describes the propagation of mesons and baryons
- ▶ Invariant under global $\mathbb{Z}(3)$ -transformations
- ▶ Description in terms of (anti-)quark occupation numbers $n_{\bar{x}}$
- ▶ Suffers from a severe sign problem, unless
 - ▶ all $P_{\bar{x}}$ align \iff deconfined phase
 - ▶ global $\mathbb{Z}(3)$ is promoted to a local one \iff strong coupling

The 3-state Potts model in $d = 3$ dimensions

- ▶ We use the **3-state Potts model** as a proxy for the effective Polyakov loop action of **heavy-dense QCD**.

- ▶ Grand-canonical partition function of the Potts model:

$$Z_{\text{GC}}(h) = \int \mathcal{D}z \exp(-S[z] + h \sum_x z_x)$$

- ▶ **Polyakov loops** are represented by the **Potts spins** $z_x \in \mathbb{Z}(3)$
- ▶ standard nearest-neighbour interaction

$$S[z] = -\gamma \sum_{\langle xy \rangle} \delta_{z_x, z_y}$$

- ▶ external 'magnetic' field $h = (2\kappa e^\mu)^\beta \Rightarrow$ breaks $\mathbb{Z}(3)$
- ▶ There is a **sign problem** for $h \neq 0$, i.e. at finite quark density.

The 3-state Potts model in $d = 3$ dimensions

- ▶ Canonical partition function for N_Q quarks:

$$Z_C(N_Q) = \sum_{\{n\}, |n|=N_Q} \int \mathcal{D}z \exp(-S[z]) \cdot \prod_x f[z_x, n_x]$$

- ▶ local quark occupation number $n_x \leq n_x^{\max}$ with $|n| = N_Q$
- ▶ use the simple local fermionic weights

$$f[z, n] = z^n$$

- ▶ equivalent to the grand-canonical partition function for small h
i.e. small density:

$$Z_{GC}(h) \simeq \sum_{N_Q=0}^{\infty} e^{\mu N_Q} Z_C(N_Q) \quad \text{for } h = e^{\mu} \ll 1$$

The 3-state Potts model in $d = 3$ dimensions

Canonical partition function

$$Z_C(N_Q) = \sum_{\{n\}} \int \mathcal{D}z \exp(\gamma \sum_{\langle xy \rangle} \delta_{z_x, z_y}) \prod_x z_x^{n_x}$$

- ▶ Action is manifestly complex \Rightarrow fermion sign problem!
- ▶ Global $\mathbb{Z}(3)$ symmetry ensures $Z_C(N_Q \neq 0 \bmod 3) = 0$:
 - ▶ projection onto integer baryon numbers
- ▶ In the limit $\gamma \rightarrow 0$, the global $\mathbb{Z}(3)$ becomes a local one:
 - ▶ projection onto integer baryon numbers on single sites

$$n_x = 0 \bmod 3 \quad (\text{limit } \gamma \rightarrow 0)$$

- ▶ sign problem is absent

Bond formulation and cluster algorithm

- ▶ Introduce bonds to express the action as

$$e^{\gamma \cdot \delta_{z_x, z_y}} = \sum_{b_{xy}=0}^1 (\delta_{z_x, z_y} \delta_{b_{xy}, 1} (e^\gamma - 1) + \delta_{b_{xy}, 0})$$

- ▶ The canonical partition function now becomes

$$Z_C(N_Q) = \sum_{\{n\}} \sum_{\{b\}} \int \mathcal{D}z \prod_{\langle xy \rangle} (\delta_{z_x, z_y} \delta_{b_{xy}, 1} (e^\gamma - 1) + \delta_{b_{xy}, 0}) \prod_x z_x^{n_x}$$

- ▶ **sum over all bond configurations $\{b\}$**

- ▶ Define the sum of bond weights over $\{n\}, \{b\}, \mathcal{D}z$ as $\langle\langle \cdot \rangle\rangle_{N_Q}$:

$$Z_C(N_Q) = \langle\langle \prod_x z_x^{n_x} \rangle\rangle_{N_Q}$$

Bond formulation and cluster algorithm

- ▶ $N_Q = 0$ gives the usual **Swendsen-Wang cluster construction**:
 - ▶ bond b_{xy} is occupied with probability $p(b_{xy} = 1) = (e^\gamma - 1)$, if $z_x = z_y$
 - ▶ weight of bond configuration is $W(\{b\}) = (e^\gamma - 1)^{N_b}$, with $N_b = \sum_{\langle xy \rangle} b_{xy}$
- ▶ Summation over $\mathbb{Z}(3)$ spins within connected cluster yields

$$Z_C(N_Q = 0) = \langle\langle 1 \rangle\rangle_{N_Q=0} = \sum_{\{b\}} (e^\gamma - 1)^{N_b} \cdot 3^{N_C}$$

- ▶ **total number of clusters N_C**
- ▶ cluster algorithm requires Euler-tour trees to achieve dynamic connectivity in $\mathcal{O}(\ln^2 V)$ instead of $\mathcal{O}(V \ln V)$ or $\mathcal{O}(V^2)$

Solution of the sign problem in the canonical formulation

- ▶ In the canonical formulation the cluster algorithm solves the sign problem:
 - ▶ include the fermionic contribution with an **improved estimator**
 - ▶ similar to idea in the grand canonical formulation

[Alford, Chandrasekharan, Cox, Wiese 2001]
- ▶ Average $\prod_x z_x^{n_x}$ over the subensemble of the 3^{N_C} configurations related by the $\mathbb{Z}(3)$ transformations:
 - ▶ total weight can be factorized into individual cluster weights $W_0(C)$,

$$\left[\prod_x z_x^{n_x} \right]_{3^{N_C}} = \left[\prod_C \prod_{x \in C} z_x^{n_x} \right]_{3^{N_C}} = \prod_C \left[\prod_{x \in C} z_x^{n_x} \right]_3 = \prod_C W_0(C)$$

where

$$W_0(C) = \left[\prod_{x \in C} z_x^{n_x} \right]_3 = \left[z^{\sum_{x \in C} n_x} \right]_3 = \begin{cases} 1 & \text{if } \sum_{x \in C} n_x = 0 \pmod{3}, \\ 0 & \text{else.} \end{cases}$$

Solution of the sign problem in the canonical formulation

- ▶ Hence, the canonical partition function becomes

Sign free canonical partition function

$$Z_C(N_Q) = \langle\langle \prod_x z_x^{n_x} \rangle\rangle_{N_Q} = \sum_{\{n\}} \sum_{\{b\}} (e^\gamma - 1)^{N_b} \cdot 3^{N_C} \cdot \prod_C \delta_{n_C, 0}$$

- ▶ $n_C = \sum_{x \in C} n_x \bmod 3$ denotes the **triality of the cluster C**
- ▶ $\prod_C \delta_{n_C, 0}$ projects on sector of configurations with triality-0 clusters only
- ▶ An intuitive, physical picture emerges:
 - ▶ only clusters with integer baryon number contribute
⇒ **confinement**
 - ▶ quarks can move freely within the cluster
⇒ **deconfinement within cluster**

Improved estimators for physical quantities

- ▶ We can define an improved estimator for the quark-antiquark correlator:

$$\langle z_x z_y^* \rangle_{N_Q} \equiv \langle\langle z_x z_y^* \prod_w z_w^{n_w} \rangle\rangle_{N_Q} / \langle\langle \prod_{w \in C} z_w^{n_w} \rangle\rangle_{N_Q}$$

- ▶ First calculate weight for cluster C containing source z_y^* :

$$\left[\prod_{w \in C} z_w^{n_w - \delta_{w,y}} \right]_3 = \left[z^{\sum_{w \in C} n_w - \delta_{w,y}} \right]_3 = \left\{ \begin{array}{ll} 1 & \text{if } \sum_{w \in C} n_w = 1 \pmod{3} \\ 0 & \text{else} \end{array} \right\} = \delta_{n_C, 1}$$

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- ▶ ... and the weight for cluster C containing source z_x :

$$\left[\left[\prod_{w \in C} z_w^{n_w + \delta_{w,x}} \right] \right]_3 = \left[\left[z^{\sum_{w \in C} n_w + \delta_{w,x}} \right] \right]_3 = \left\{ \begin{array}{ll} 1 & \text{if } \sum_{w \in C} n_w = 2 \pmod{3} \\ 0 & \text{else} \end{array} \right\} = \delta_{n_C, 2}$$

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- ▶ Calculate the subensemble average including $z_x z_y^*$:

$$\begin{aligned} \left[\left[z_x z_y^* \prod_w z_w^{n_w} \right] \right]_{3^{N_C}} &= \delta_{C_x, C_y} \cdot \left[\left[z_x z_y^* \prod_w z_w^{n_w} \right] \right]_{3^{N_C}} \\ &+ (1 - \delta_{C_x, C_y}) \cdot \left[\left[z_x z_y^* \prod_w z_w^{n_w} \right] \right]_{3^{N_C}} \end{aligned}$$

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Improved estimators for physical quantities

- ▶ Similar expressions for $z_x z_y$, $z_x^* z_y^*$, z_x , $z_x^* = z_x^2$, ...

- ▶ An interesting quantity is the the **quark chemical potential**:

$$\mu(\rho) \equiv -\frac{1}{3} \log \frac{Z_C(N_Q + 3)}{Z_C(N_Q)}$$

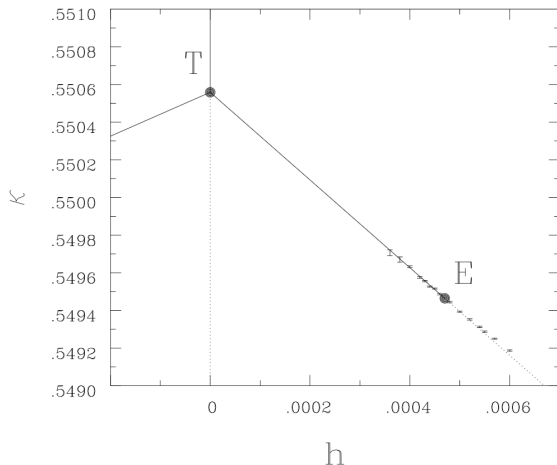
- ▶ quark density $\rho \equiv (N_Q + 3/2)/V$
- ▶ The expectation value of the phase of $Z(N_Q)$:

$$\ln \langle \exp(i\phi) \rangle_{|\cdot|, N_Q} = \frac{\langle \langle \prod_x z_x^{n_x} \rangle \rangle_{N_Q}}{\langle \langle 1 \rangle \rangle_{N_Q}} = -3 \sum_{k=0}^{N_Q/3-1} \mu\left(\frac{3}{2} + 3k\right) - \ln \mathcal{P}(N_Q, V)$$

Physics of the 3-state Potts model

- Phase diagram in the $(e^\mu, \gamma) \equiv (h, \kappa)$ -plane:

[Alford, Chandrasekharan, Cox and Wiese 2001]

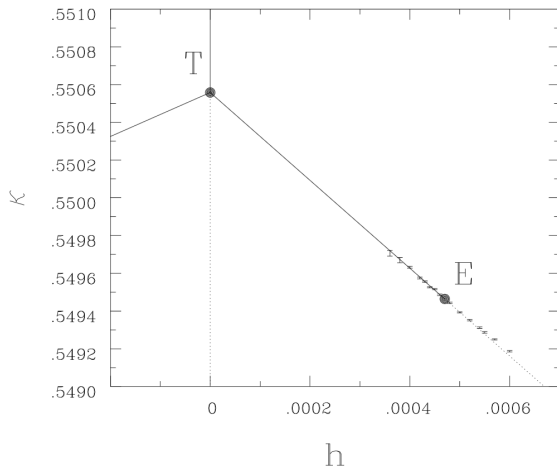


- deconfinement phase transition at $T = (0, 0.550565(10))$

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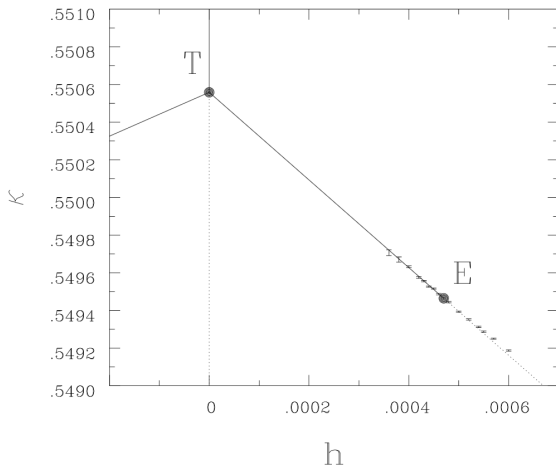


- line of first order phase transitions from T to E

Physics of the 3-state Potts model

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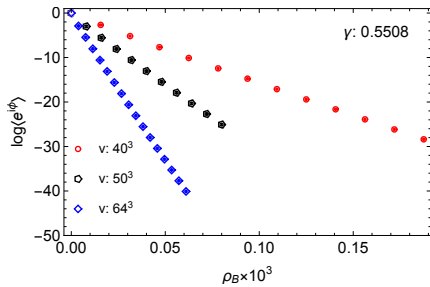
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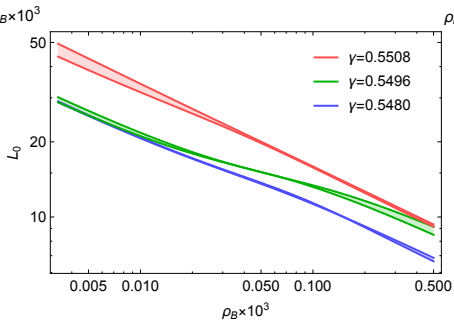
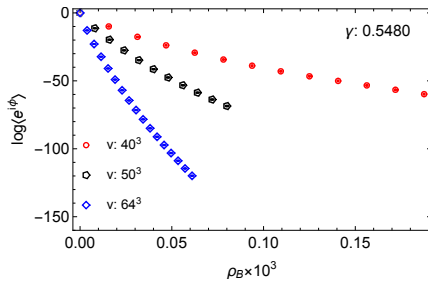
- critical endpoint $E = (0.000470(2), 0.549463(13))$

Severity of the sign problem

Deconfined phase:

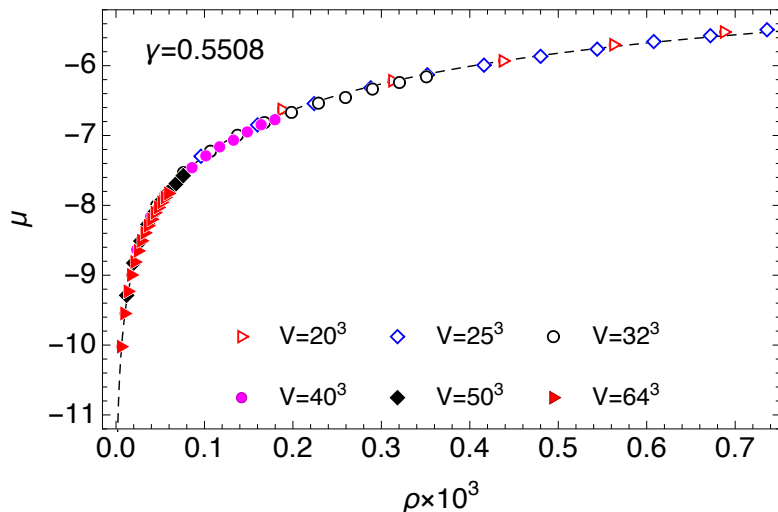


Confined phase:



Physics of the 3-state Potts model

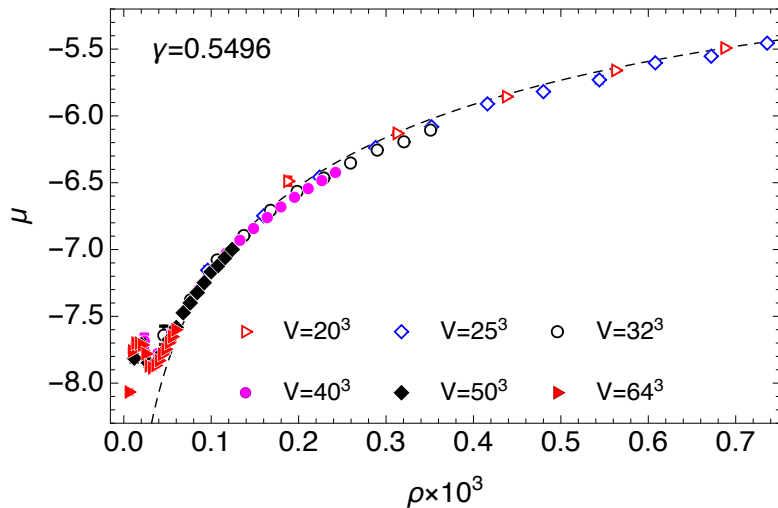
- ▶ Canonical simulation results in the deconfined phase:



- ▶ description in terms of a gas of (free) quarks

Physics of the 3-state Potts model

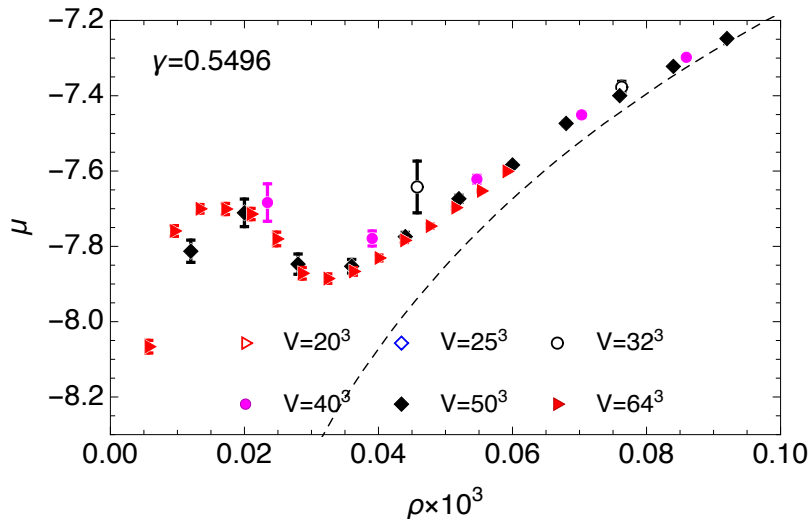
- ▶ Results from below the deconfinement transition:



- ▶ transition from the confined into the deconfined phase

Physics of the 3-state Potts model

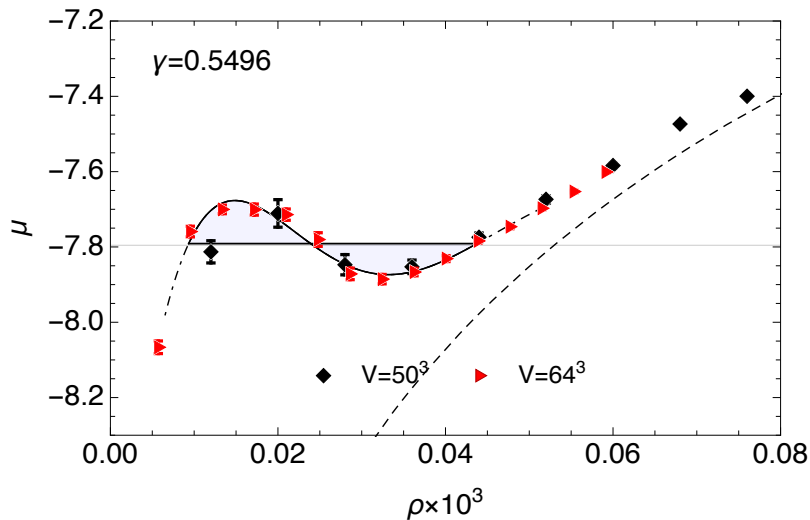
- ▶ Results from below the deconfinement transition:



- ▶ typical signature of a 1st order phase transition

Physics of the 3-state Potts model

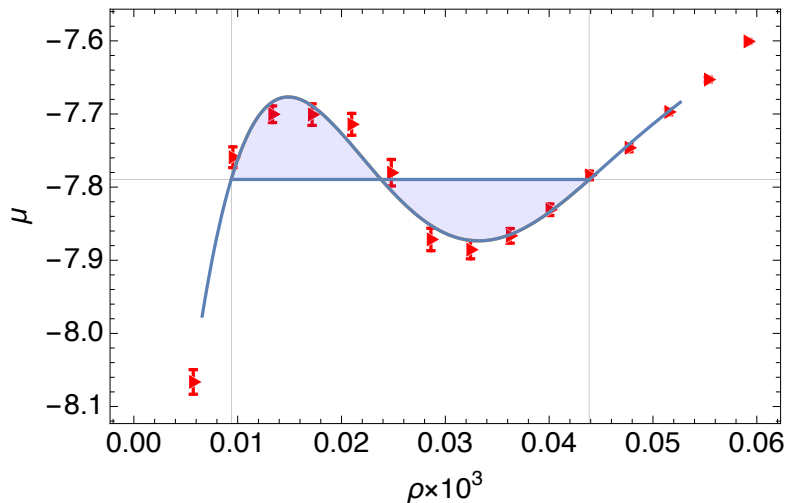
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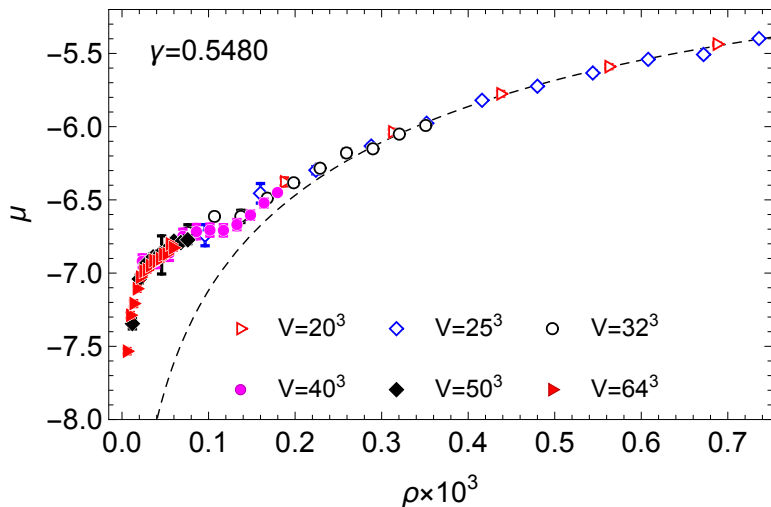
- ▶ Results from below the deconfinement transition:



- ▶ Maxwell construction yields critical μ_c

Physics of the 3-state Potts model

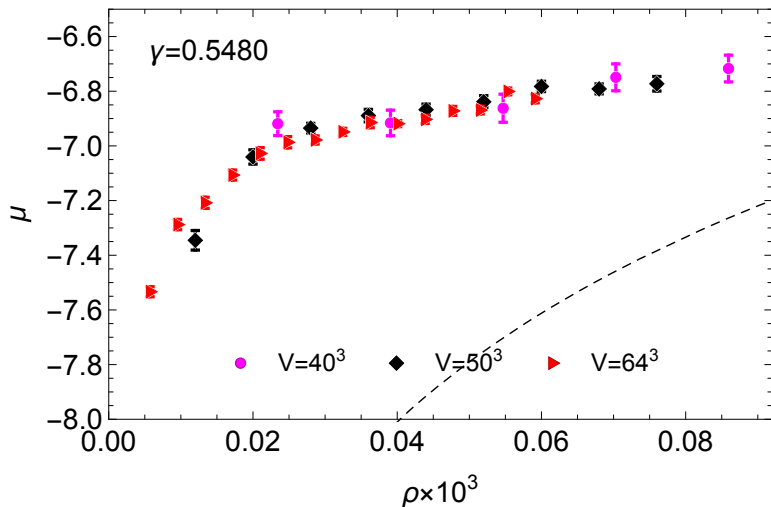
- ▶ Results from below the critical endpoint:



- ▶ crossover from the confined into the deconfined phase

Physics of the 3-state Potts model

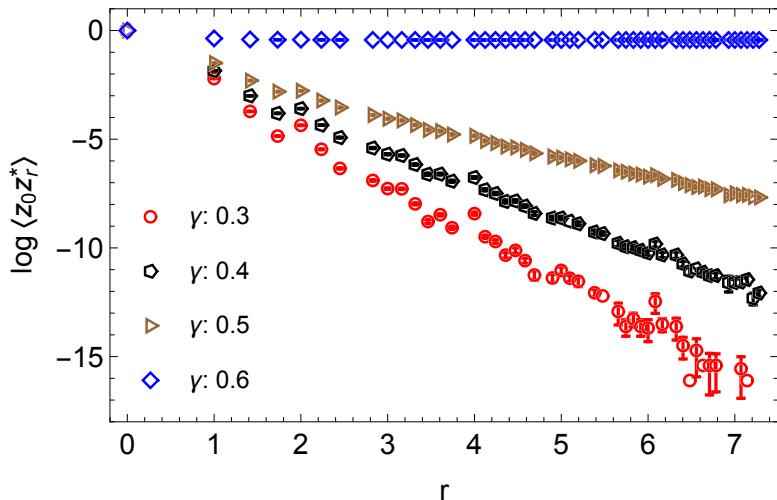
- ▶ Results from below the critical endpoint:



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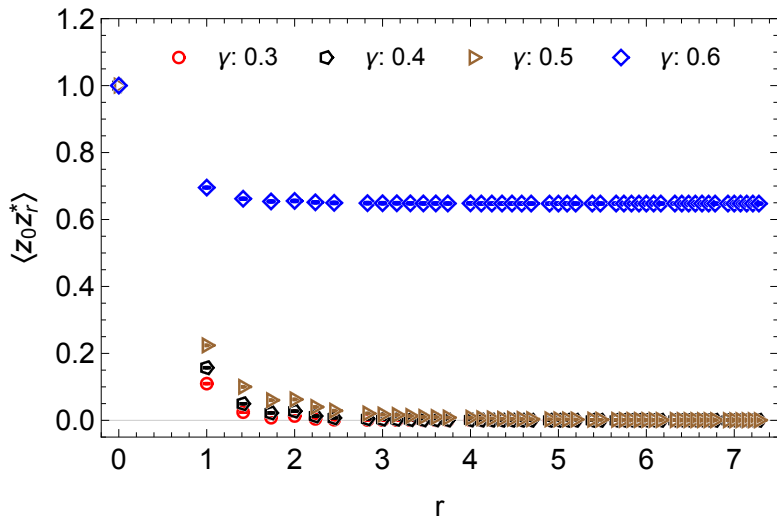
Physics of the 3-state Potts model

- ▶ (Anti)Quark-(anti)quark potentials at zero density:



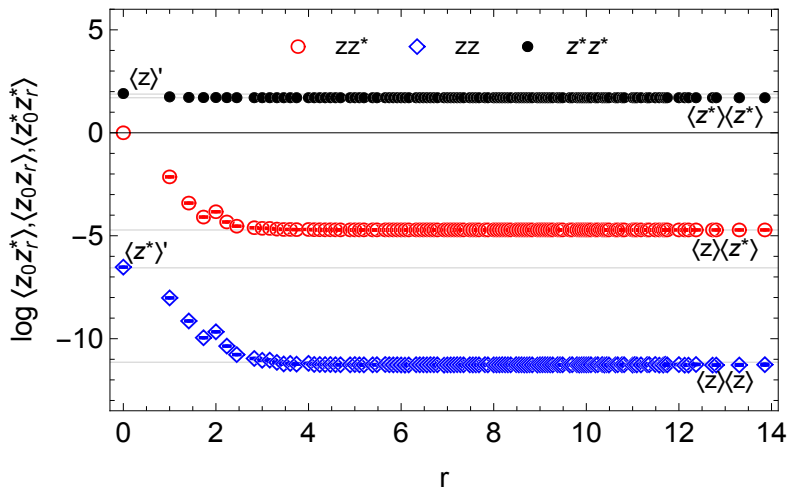
Physics of the 3-state Potts model

- ▶ (Anti)Quark-(anti)quark potentials at zero density:



Physics of the 3-state Potts model

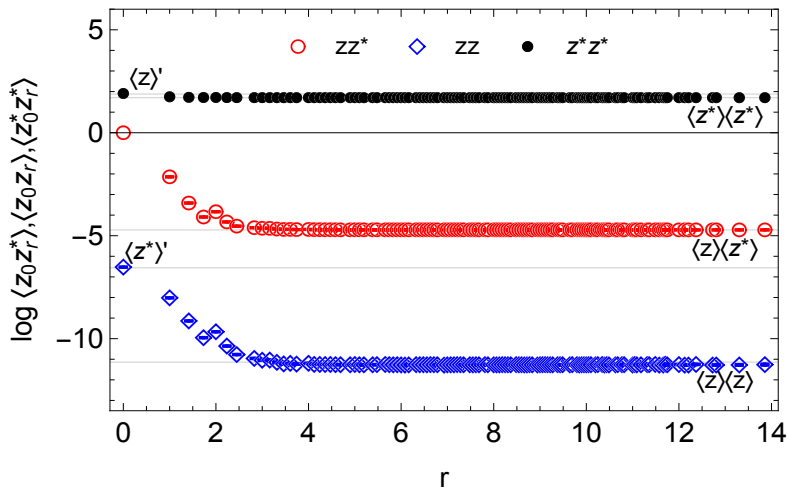
- ▶ (Anti)Quark-(anti)quark potentials at low temperature:



- ▶ confined phase: $\gamma = 0.3$ for $N_Q = 24$, $V = 16^3$, i.e. $\rho = 5.9 \cdot 10^{-3}$

Physics of the 3-state Potts model

- ▶ (Anti)Quark-(anti)quark potentials at low temperature:



- ▶ values at $r = 0$ and $r \rightarrow \infty$ match $\langle z \rangle, \langle z^* \rangle, \langle z^* \rangle \langle z^* \rangle, \dots$

Conclusions

- ▶ We solved the fermion sign problem for the $\mathbb{Z}(3)$ Potts model
 - ▶ isolate coherent dynamics of the $\mathbb{Z}(3)$ spins in clusters
 - ▶ cluster subaverages project on **nonzero, positive contributions**
⇒ increase of statistics exponential in N_C
- ▶ The solution provides an **appealing physical picture**:
 - ▶ quarks confined in clusters, but move freely within
 - ▶ at $\gamma \rightarrow 0$ clusters are confined to single sites only
 - ▶ **deconfinement** corresponds to appearance of a **percolating cluster**

Good algorithms reflect true physics insight!

- ▶ Extension to Polyakov loop models could be possible:
 - ▶ mechanism at work at $\beta = 0$
 - ▶ extend it to $\beta > 0$ ⇒ $\mathbb{Z}(N_c)$ clusters for gauge fields