Solution of the sign problem in the Potts model at fixed baryon number
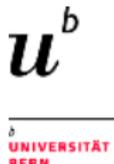
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Lattice 2017

Motivation: QCD in the heavy-dense limit

‣ Effective action in terms of (anti-)Polyakov loops P and $P^\dagger$.

‣ Canonical determinant $n_f = 3$ quarks:

$$\det \mathcal{D}^{HD}_{n_f=3} \sim 2\sum_{\bar{x}}(\operatorname{Tr} P_{\bar{x}})^2 \sum_{\bar{y}} \operatorname{Tr} P_{\bar{y}} + 4\sum_{\bar{x}} \operatorname{Tr} P_{\bar{x}} \sum_{\bar{y}\neq\bar{x}} \operatorname{Tr} P_{\bar{y}} \sum_{\bar{z}} \operatorname{Tr} P_{\bar{z}}$$

  ‣ describes the propagation of baryons

‣ Invariant under global $\mathbb{Z}(3)$-transformations

‣ 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

Outline

- 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]

- Physics of the 3-state Potts model
  - Density driven phase transition
  - (Anti-)Quark-(anti-)Quark correlators

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

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

- 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 $\gamma \to 0$, the global $\mathbb{Z}(3)$ becomes a local one:
  - projection onto integer baryon numbers on single sites

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

  - sign problem is absent

Bond formulation and cluster algorithm

▸ Introduce bonds to express the action as

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

▸ The canonical partition function now becomes

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

  ▸ sum over all bond configurations $\{b\}$

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

$$Z_C(N_Q) = \left\langle\!\!\left\langle \prod_{x} z_x^{n_x} \right\rangle\!\!\right\rangle_{N_Q}$$

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 $W_0(C)$,

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

where

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

Solution of the sign problem in the canonical formulation

‣ Hence, the canonical partition function becomes

Sign free canonical partition function

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

‣ $n_C = \sum_{x \in C} n_x \bmod 3$ 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
        $\Rightarrow$ confinement
  ‣ quarks can move freely within the cluster
        $\Rightarrow$ 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^*:

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

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▸ ... and the weight for cluster C containing source z_x:

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

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

$$\left[\!\left[z_x z_y^* \prod_w z_w^{n_w} \right]\!\right]_{3^{N_C}} = \delta_{C_x, C_y} \cdot \left[\!\left[z_x z_y^* \prod_w z_w^{n_w} \right]\!\right]_{3^{N_C}}$$

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

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$$+ (1 - \delta_{C_x, C_y}) \cdot \delta_{n_{C_x}, 2} \cdot \delta_{n_{C_y}, 1} \prod_{\substack{C \neq C_x \\ C \neq C_y}} \delta_{n_C, 0}$$

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 $\rho \equiv (N_Q + {}^3/_2)/V$
  - partition function ratio can be computed using the multiplicity ratio average

$$\frac{Z_C(N_Q + 3)}{Z_C(N_Q)} = \left\langle \frac{\mathcal{M}(N_Q + 3, \{b\})}{\mathcal{M}(N_Q, \{b\})} \right\rangle_{N_Q}$$

  and an estimator for the multiplicity ratio.

Physics of the 3-state Potts model

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

  [Alford, Chandrasekharan, Cox and Wiese 2001]
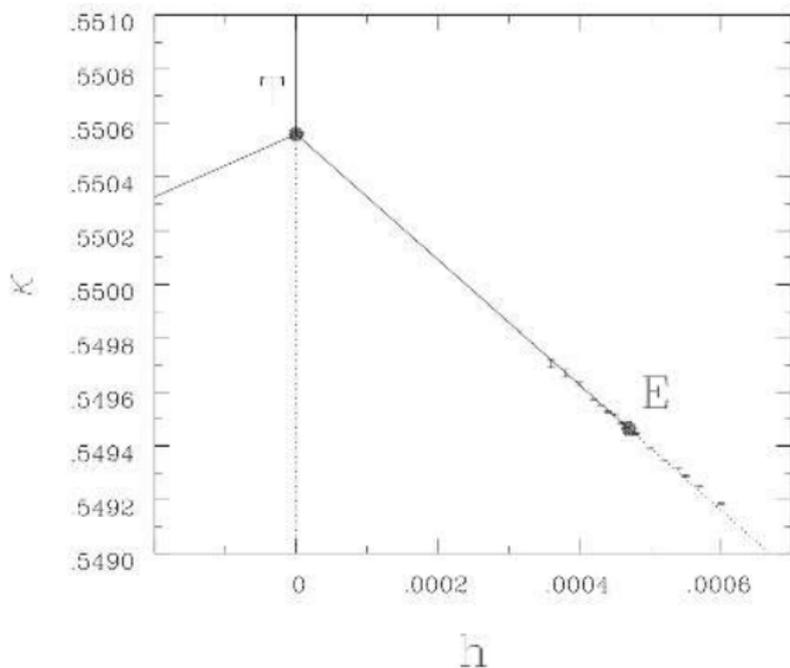
- deconfinement phase transition at $T = (0, 0.550565(10))$

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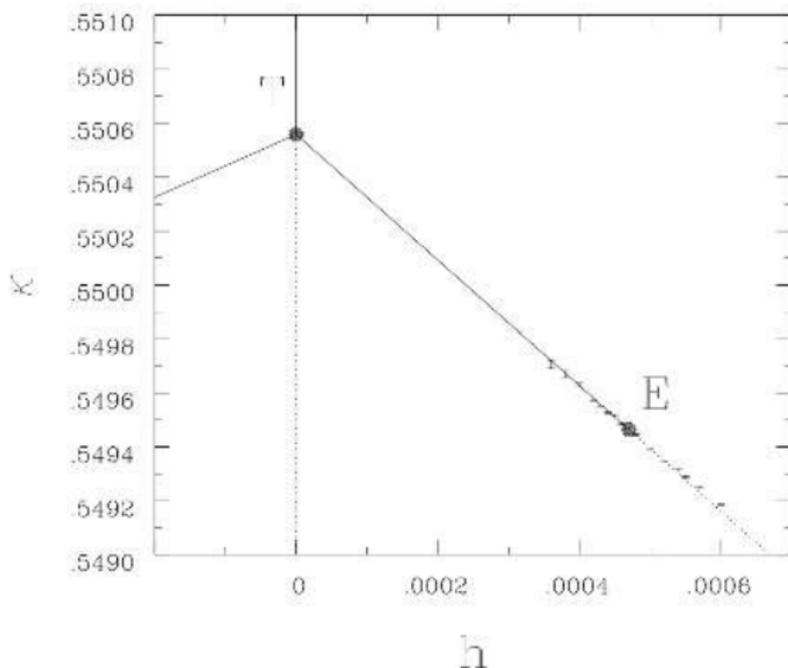
‣ line of first order phase transitions from T to E

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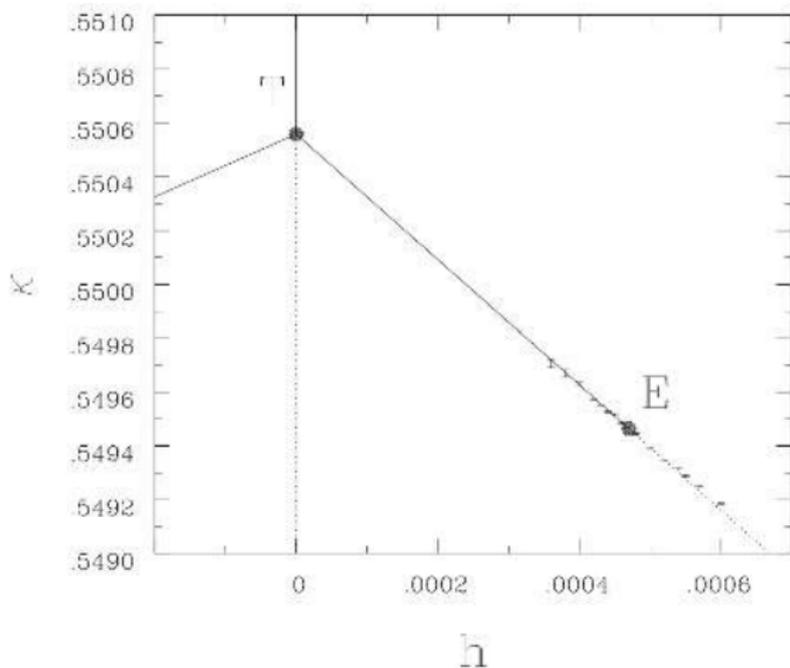
‣ critical endpoint $E = (0.000470(2), 0.549463(13))$

Physics of the 3-state Potts model

‣ Canonical simulation results in the deconfined phase:
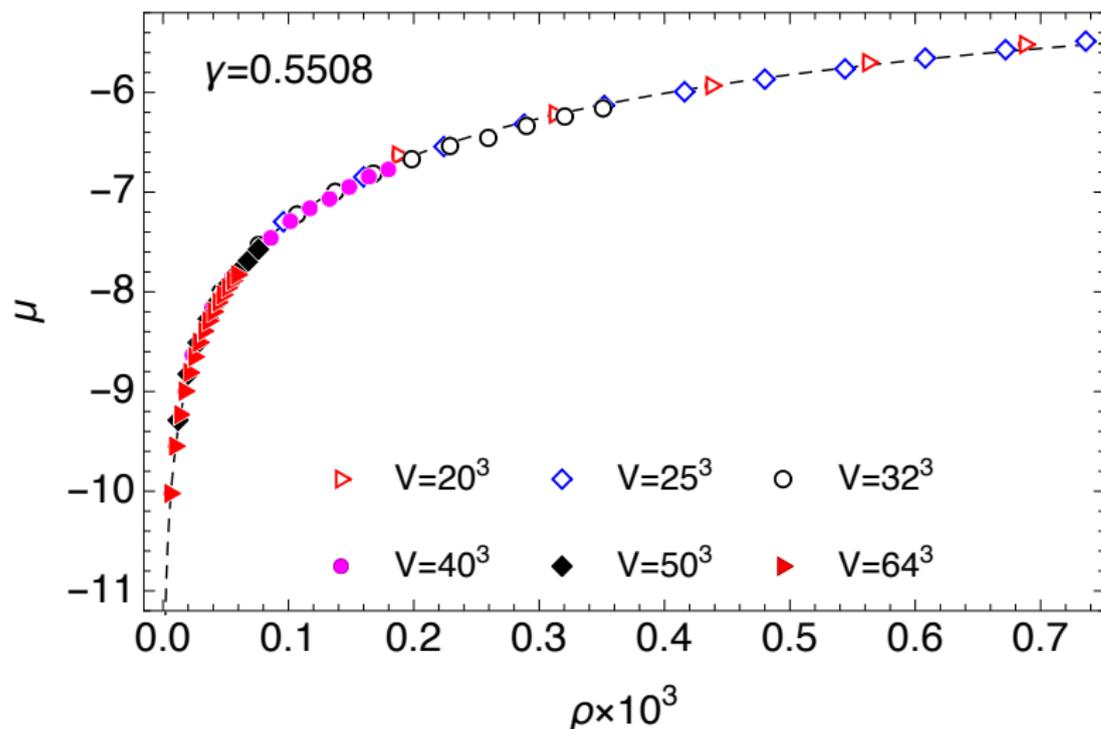
‣ description in terms of a gas of (free) quarks

Physics of the 3-state Potts model

‣ Results from below the deconfinement transition:
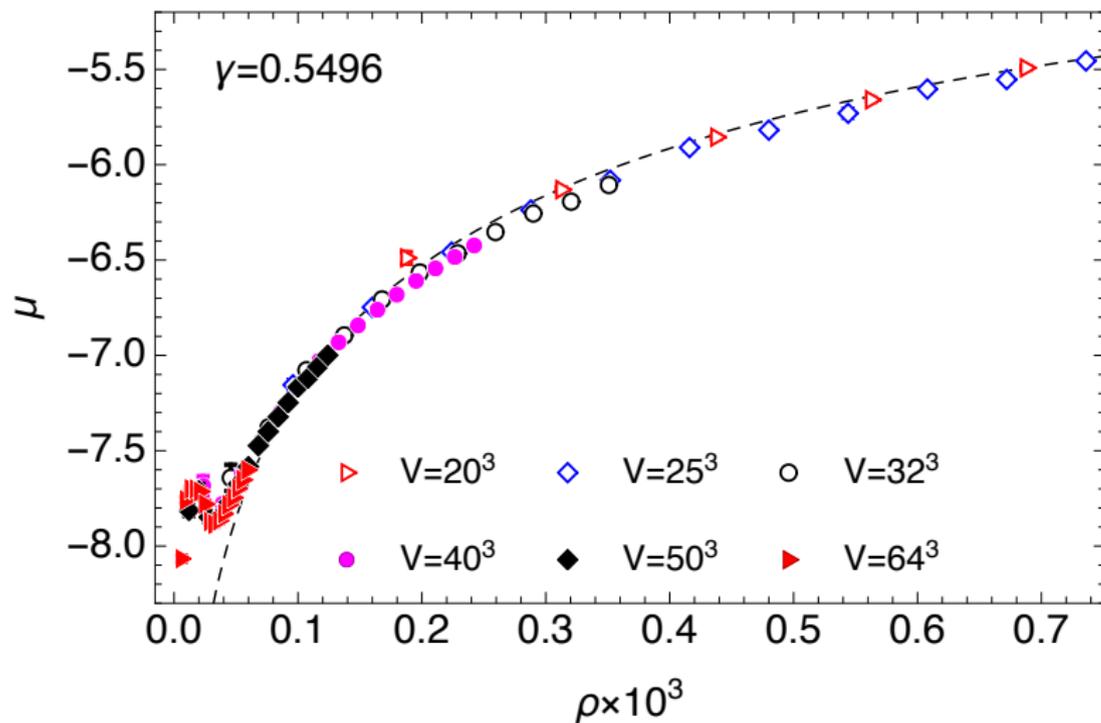
‣ transition from the confined into the deconfined phase

Physics of the 3-state Potts model

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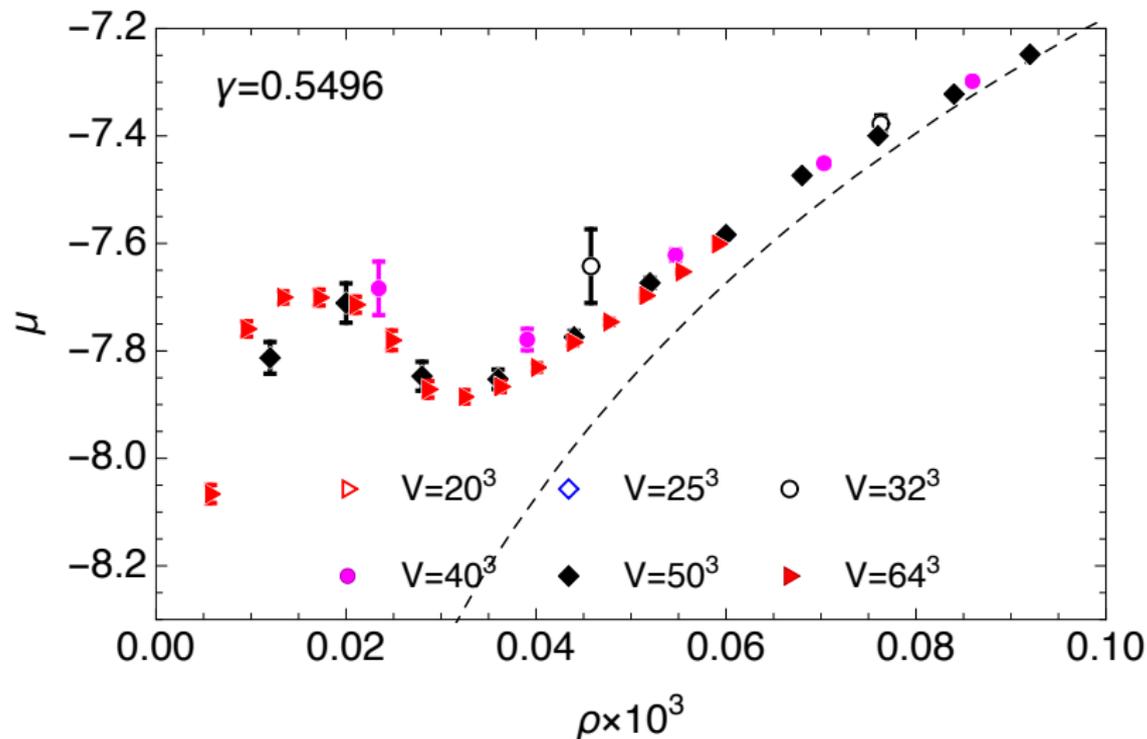
‣ typical signature of a 1st order phase transition
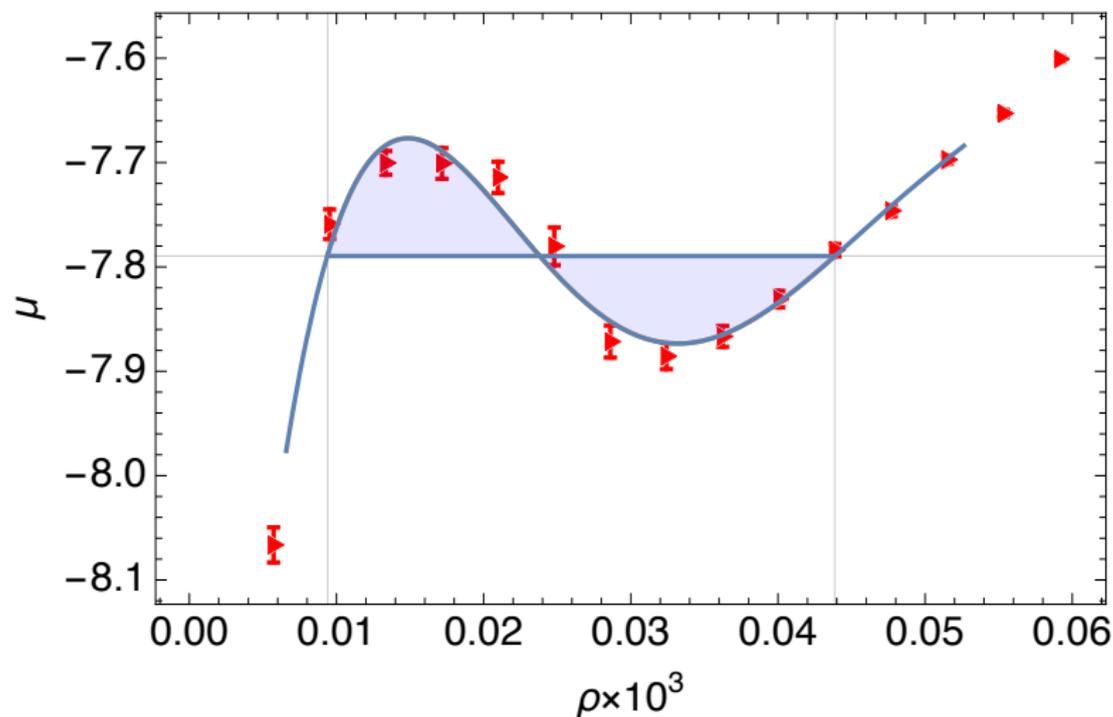
Physics of the 3-state Potts model
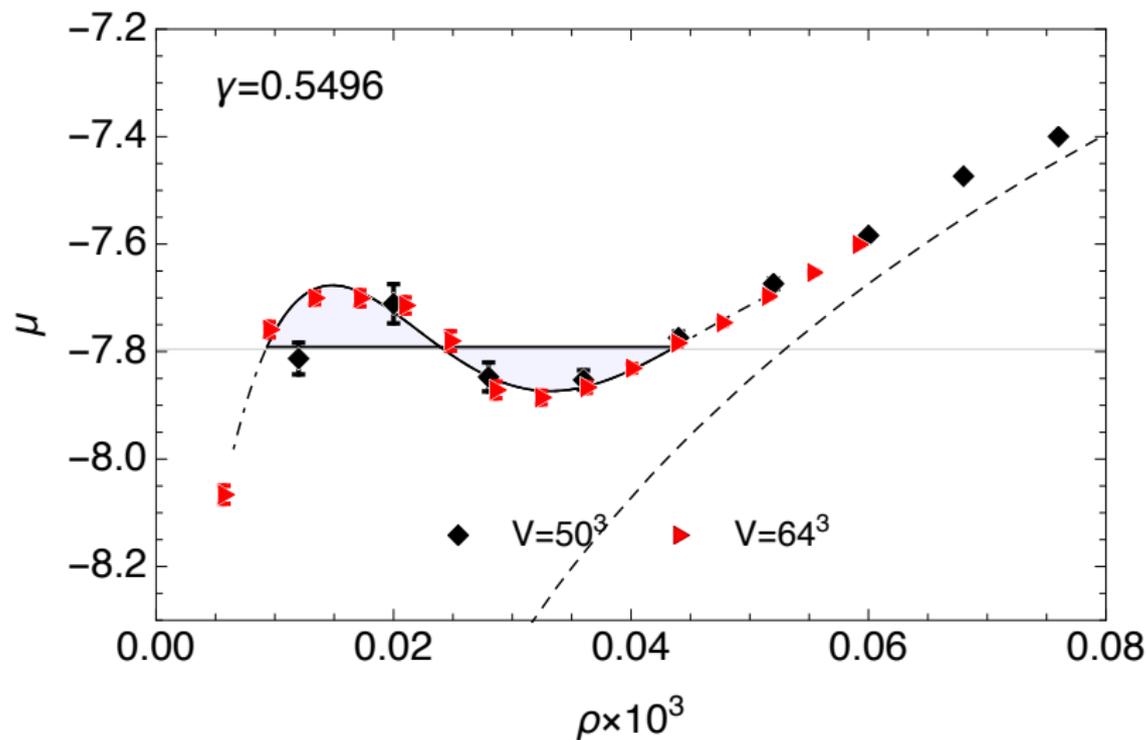
▸ Results from below the deconfinement transition:

▸ Maxwell construction yields critical μ_c

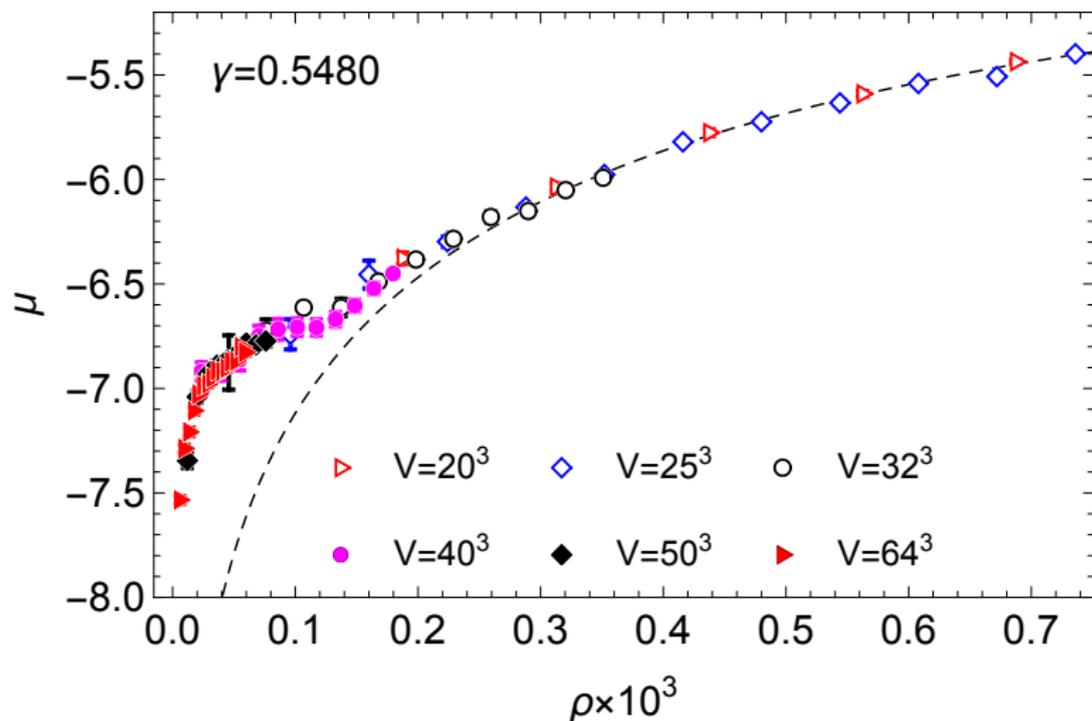# Physics of the 3-state Potts model

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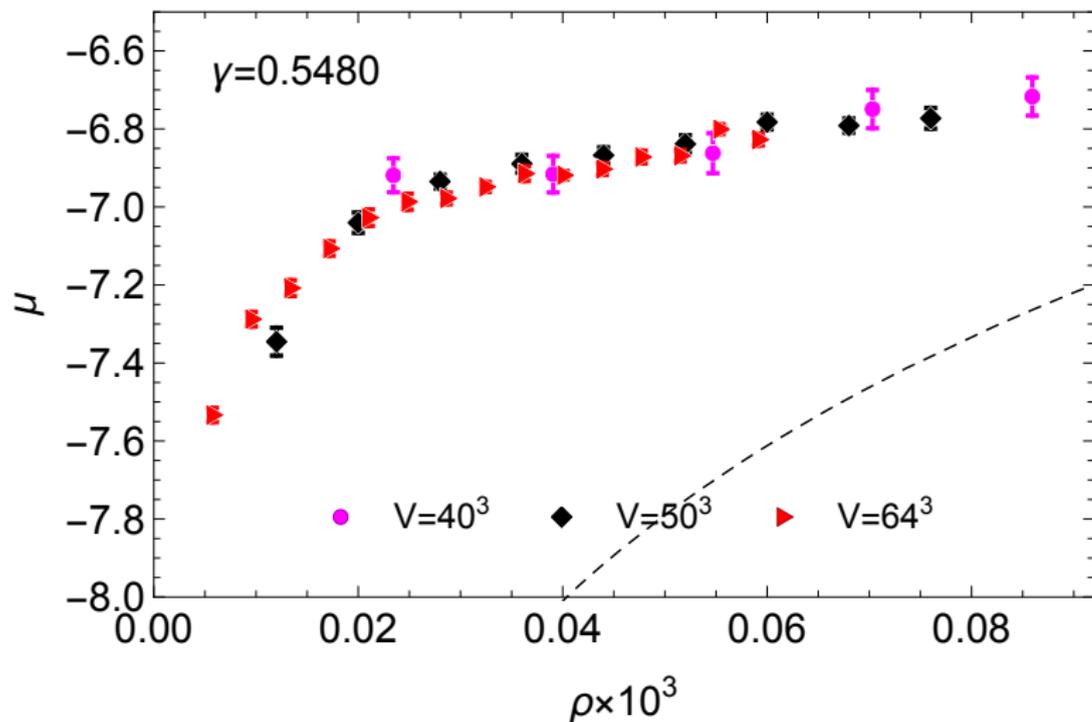
Physics of the 3-state Potts model

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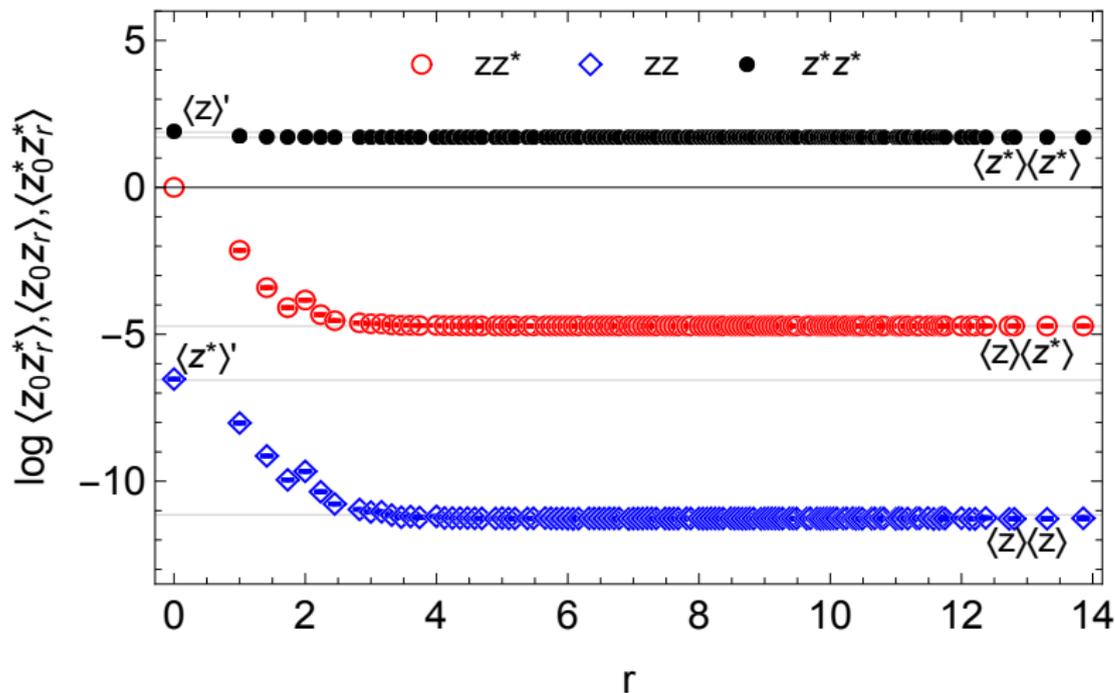
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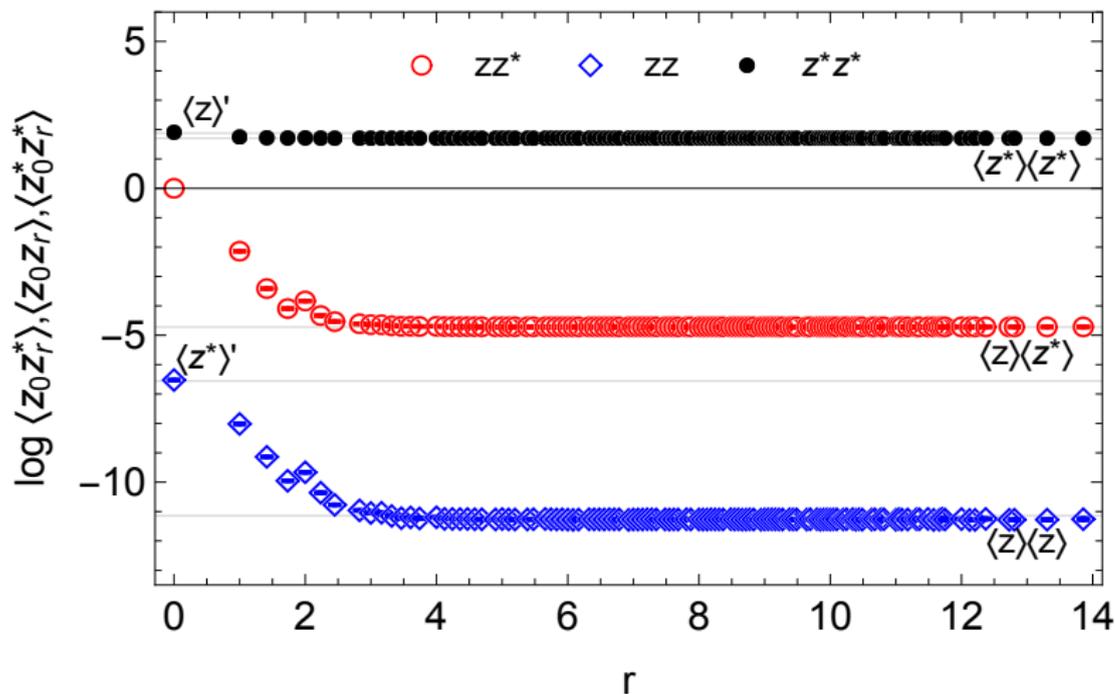
Physics of the 3-state Potts model

▸ (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 $r \to \infty$ match $\langle z \rangle$, $\langle z^* \rangle$, $\langle z^* \rangle \langle z^* \rangle$, ...

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
    $\Rightarrow$ increase of statistics exponential in N_C

- The solution provides an appealing physical picture:

> Good algorithms reflect true physics insight! [Neuberger '17]

  - quarks confined in clusters, but move freely within
  - at $\gamma \to 0$ clusters are confined to single sites only
  - deconfinement corresponds to appearance of a percolating cluster

- Extension to Polyakov loop models could be possible:
  - mechanism at work at $\beta = 0$
  - extend it to $\beta > 0$

Motivation: QCD in the heavy-dense limit

- ▸ Allows to describe static quarks and anti-quarks.

- ▸ Effective action in terms of Polyakov loops P and anti-Polyakov loops $P^\dagger$ in $d = 3$:

Fermion determinant for $N_f = 2$ QCD

$$\det \mathcal{D}_a^{HD} = \prod_{\bar{x}} \det \left[\mathbb{I} + (2\kappa e^{+\mu})^{L_t} P_{\bar{x}} \right]^2 \det \left[\mathbb{I} + (2\kappa e^{-\mu})^{L_t} P_{\bar{x}}^\dagger \right]^2$$

- ▸ Canonical determinants obtained from transfer matrices.

Motivation: QCD in the heavy-dense limit

▸ Canonical determinant describing a single quark, i.e. $n_f = 1$:

$$\det \mathcal{D}_{n_f=1}^{HD} = \left((2\kappa)^{L_t} + (2\kappa)^{-L_t}\right) \cdot \sum_{\bar{x}} \operatorname{Tr} P_{\bar{x}}$$

▸ For $n_f = 2$ quarks:

$$\det \mathcal{D}_{n_f=2}^{HD}/\Omega \propto 2 \sum_{\bar{x}} \operatorname{Tr} P_{\bar{x}} \sum_{\bar{y}} \operatorname{Tr} P_{\bar{y}}$$

$$+ \left(4 \sum_{\bar{x}} \operatorname{Tr} P_{\bar{x}} \sum_{\bar{y}} \operatorname{Tr} P_{\bar{y}} - 3 \sum_{\bar{x}} \left(\operatorname{Tr} P_{\bar{x}}\right)^2 + 2 \operatorname{Tr} P_{\bar{x}}^{\dagger}\right)$$

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

Motivation: QCD in the heavy-dense limit

▸ Canonical determinant $n_f = 3$ quarks:

$$\det \mathcal{D}^{HD}_{n_f=3}/\Omega = h_3 \cdot \left(4\sum_{\bar{x}} \operatorname{Tr} P^\dagger_{\bar{x}} \sum_{\bar{y}} \operatorname{Tr} P_{\bar{y}} - 3\sum_{\bar{x}} \operatorname{Tr} P_{\bar{x}} \operatorname{Tr} P^\dagger_{\bar{x}} + 2L^3_s \right)$$

$$+ h_1 \left(4\sum_{\bar{x}} \operatorname{Tr} P^\dagger_{\bar{x}} \sum_{\bar{y}} \operatorname{Tr} P_{\bar{y}} + 2\sum_{\bar{x}} (\operatorname{Tr} P_{\bar{x}})^2 \sum_{\bar{y}} \operatorname{Tr} P_{\bar{y}} \right.$$

$$\left. + 4\sum_{\bar{x}} \operatorname{Tr} P_{\bar{x}} \sum_{\bar{y}\neq\bar{x}} \operatorname{Tr} P_{\bar{y}} \sum_{\bar{z}} \operatorname{Tr} P_{\bar{z}} \right)$$

   ▸ describes the propagation of mesons and baryons

▸ Invariant under global $\mathbb{Z}(3)$-transformations

▸ 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