

Exploring the QCD phase diagram via reweighting from isospin chemical potential

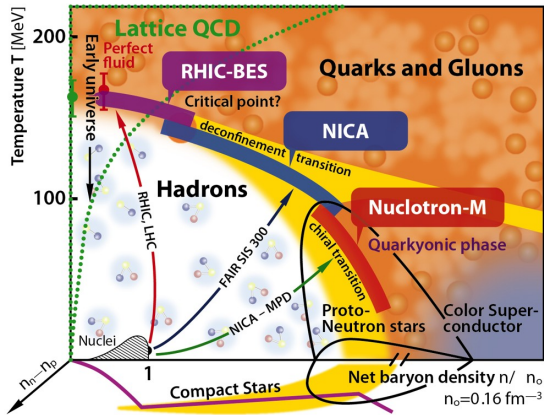
Sebastian Schmalzbauer

in collaboration with B. Brandt, F. Cuteri, G. Endrődi



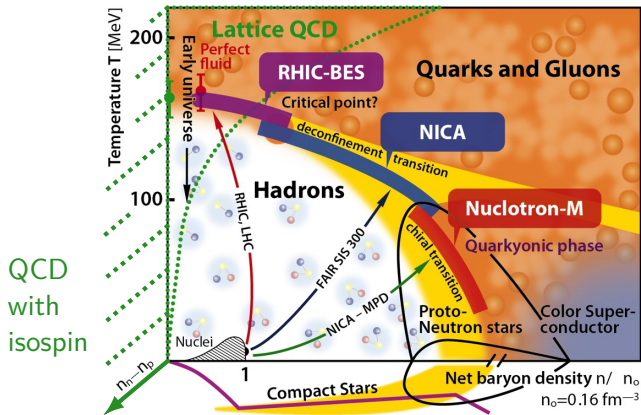
- introduction
 - QCD with isospin asymmetry: phase diagram
 - (spontaneous) symmetry breaking, pion condensation
- dependence of phase boundary on chemical potentials
 - reweighting to $\mu_S > 0$
 - reweighting to $\mu_B > 0$
- decoupling of auxiliary quarks
 - reweighting in m_q
- summary & outlook

QCD phase diagram



(taken from NICA)

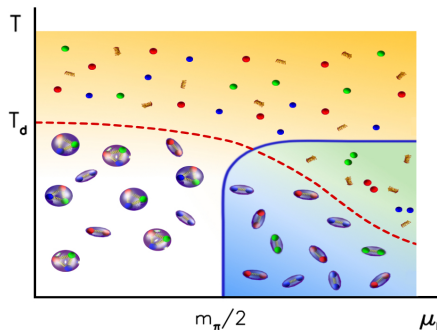
QCD phase diagram



(taken from NICA)

QCD isospin phase diagram

- baryon chemical potential $\mu_B = 0$
- **isospin chemical potential** $\mu_I = (\mu_u - \mu_d)/2$
- rich phase structure: [B. Brandt, G. Endrödi, S. Schmalzbauer '18]
 - vacuum (white)
 - quark-gluon plasma
 - pion condensate (BEC)
 - BCS phase
- dependence of BEC phase boundary on μ_B, μ_S ?



Simulation Details

- QCD partition function for $N_f = 2 + 1$ rooted staggered quarks

$$\mathcal{Z} = \int \mathcal{D}[U] (\det \mathcal{M}_{ud} \mathcal{M}_s)^{1/4} e^{-S_G}$$

- quark matrices with $\eta_5 = (-1)^{n_t+n_x+n_y+n_z}$

$$\mathcal{M}_{ud} = \begin{pmatrix} \not{D}_{\mu_l} + m_{ud} & \lambda \eta_5 \\ -\lambda \eta_5 & \not{D}_{-\mu_l} + m_{ud} \end{pmatrix}, \quad \mathcal{M}_s = \not{D}_0 + m_s$$

Simulation Details

- QCD partition function for $N_f = 2 + 1$ rooted staggered quarks

$$\mathcal{Z} = \int \mathcal{D}[U] (\det \mathcal{M}_{ud} \mathcal{M}_s)^{1/4} e^{-S_G}$$

- quark matrices with $\eta_5 = (-1)^{n_t+n_x+n_y+n_z}$

$$\mathcal{M}_{ud} = \begin{pmatrix} \not{D}_{\mu_l} + m_{ud} & \lambda \eta_5 \\ -\lambda \eta_5 & \not{D}_{-\mu_l} + m_{ud} \end{pmatrix}, \quad \mathcal{M}_s = \not{D}_0 + m_s$$

- **no sign problem** due to $\eta_5 \tau_1 \mathcal{M}_{ud} \tau_1 \eta_5 = \mathcal{M}_{ud}^\dagger$:

$$\det \mathcal{M}_{ud} = \det (M^\dagger M + \lambda^2) \in \mathbb{R}_{>0} \quad M = \not{D}_{\mu_l} + m_{ud}$$

Simulation Details

- QCD partition function for $N_f = 2 + 1$ rooted staggered quarks

$$\mathcal{Z} = \int \mathcal{D}[U] (\det \mathcal{M}_{ud} \mathcal{M}_s)^{1/4} e^{-S_G}$$

- quark matrices with $\eta_5 = (-1)^{n_t + n_x + n_y + n_z}$

$$\mathcal{M}_{ud} = \begin{pmatrix} \not{D}_{\mu_l} + m_{ud} & \lambda \eta_5 \\ -\lambda \eta_5 & \not{D}_{-\mu_l} + m_{ud} \end{pmatrix}, \quad \mathcal{M}_s = \not{D}_0 + m_s$$

- **no sign problem** due to $\eta_5 \tau_1 \mathcal{M}_{ud} \tau_1 \eta_5 = \mathcal{M}_{ud}^\dagger$:

$$\det \mathcal{M}_{ud} = \det (M^\dagger M + \lambda^2) \in \mathbb{R}_{>0} \quad M = \not{D}_{\mu_l} + m_{ud}$$

- first studies [Kogut, Sinclair '02] [de Forcrand, Stephanov, Wenger '07]
- in this work: stout-smearred quarks, physical pion masses, tree-level Symanzik improved gluons, 8^4 lattice

Pion condensation: symmetry breaking

- QCD with light quarks

$$\mathcal{M}_{ud} = \not{D} + m_{ud}$$

- chiral symmetry breaking pattern

$$SU(2)_V$$

Pion condensation: symmetry breaking

- QCD with light quarks

$$\mathcal{M}_{ud} = \not{D} + m_{ud} + \mu \gamma_0 \tau_3$$

- chiral symmetry breaking pattern

$$SU(2)_V \rightarrow U(1)_{\tau_3}$$

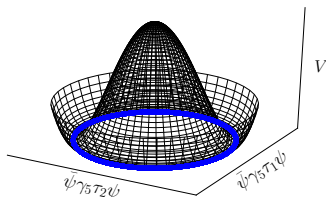
Pion condensation: symmetry breaking

- QCD with light quarks

$$\mathcal{M}_{ud} = \not{D} + m_{ud} + \mu \gamma_0 \tau_3$$

- chiral symmetry breaking pattern

$$SU(2)_V \rightarrow U(1)_{\tau_3}$$



Pion condensation: symmetry breaking

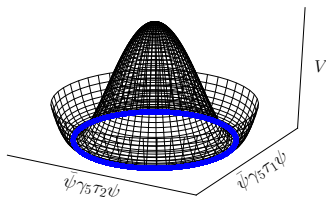
- QCD with light quarks

$$\mathcal{M}_{ud} = \not{D} + m_{ud} + \mu \gamma_0 \tau_3$$

- chiral symmetry breaking pattern

$$SU(2)_V \rightarrow U(1)_{\tau_3}$$

- **pion condensate** $\langle \bar{\psi} \gamma_5 \tau_{1,2} \psi \rangle = 0$ (finite volume)
- zero-eigenvalues: **accumulation, slowing down** (Goldstone mode)



Pion condensation: symmetry breaking

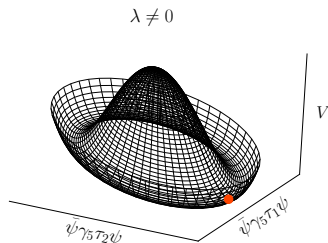
- QCD with light quarks

$$\mathcal{M}_{ud} = \not{D} + m_{ud} + \mu_1 \gamma_0 \tau_3 + i \lambda \gamma_5 \tau_2$$

- chiral symmetry breaking pattern

$$SU(2)_V \rightarrow U(1)_{\tau_3} \rightarrow \emptyset$$

- **pion condensate** $\langle \bar{\psi} \gamma_5 \tau_{1,2} \psi \rangle \neq 0$ (but unphysical value)
- zero-eigenvalues: **no, we are safe!**



Pion condensation: symmetry breaking

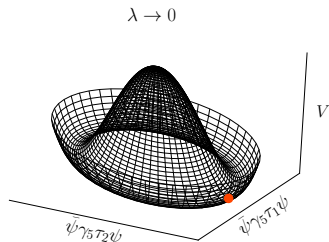
- QCD with light quarks

$$\mathcal{M}_{ud} = \not{D} + m_{ud} + \mu \not{1} \gamma_0 \tau_3 + i \lambda \not{1} \gamma_5 \tau_2$$

- chiral symmetry breaking pattern

$$SU(2)_V \rightarrow U(1)_{\tau_3} \rightarrow \emptyset$$

- **pion condensate** $\langle \bar{\psi} \not{1} \gamma_5 \tau_{1,2} \psi \rangle \neq 0$ (but unphysical value)
- zero-eigenvalues: **no, we are safe!**
- need to **extrapolate** $\lambda \rightarrow \mathbf{0}$ for physical results



Pion condensation: symmetry breaking

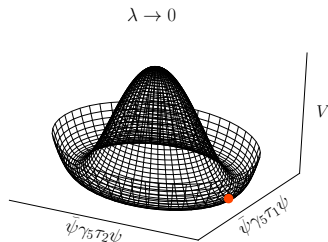
- QCD with light quarks

$$\mathcal{M}_{ud} = \not{D} + m_{ud} + \mu \not{1} \gamma_0 \tau_3 + i \lambda \not{1} \gamma_5 \tau_2$$

- chiral symmetry breaking pattern

$$SU(2)_V \rightarrow U(1)_{\tau_3} \rightarrow \emptyset$$

- **pion condensate** $\langle \bar{\psi} \not{1} \gamma_5 \tau_{1,2} \psi \rangle \neq 0$ (but unphysical value)
- zero-eigenvalues: **no, we are safe!**
- need to **extrapolate** $\lambda \rightarrow 0$ for physical results



Pion condensation: symmetry breaking

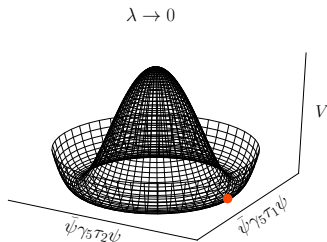
- QCD with light quarks

$$\mathcal{M}_{ud} = \not{D} + m_{ud} + \mu \not{1} \gamma_0 \tau_3 + i \lambda \not{1} \gamma_5 \tau_2$$

- chiral symmetry breaking pattern

$$SU(2)_V \rightarrow U(1)_{\tau_3} \rightarrow \emptyset$$

- **pion condensate** $\langle \bar{\psi} \not{1} \gamma_5 \tau_{1,2} \psi \rangle \neq 0$ (correct value)
- zero-eigenvalues: **no, we are safe!**
- need to **extrapolate** $\lambda \rightarrow 0$ for physical results



Pion condensation: symmetry breaking

- QCD with light quarks

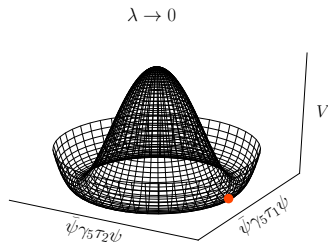
$$\mathcal{M}_{ud} = \not{D} + m_{ud} + \mu \not{1} \gamma_0 \tau_3 + i \lambda \not{5} \tau_2$$

- chiral symmetry breaking pattern

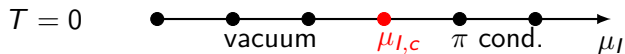
$$SU(2)_V \rightarrow U(1)_{\tau_3} \rightarrow \emptyset$$

- **pion condensate** $\langle \bar{\psi} \not{5} \tau_{1,2} \psi \rangle \neq 0$ (correct value)
- zero-eigenvalues: **no, we are safe!**
- need to **extrapolate** $\lambda \rightarrow 0$ for physical results
e.g. reweighting

$$\langle O \rangle_0 = \frac{\langle OR_\lambda \rangle_\lambda}{\langle R_\lambda \rangle_\lambda}$$

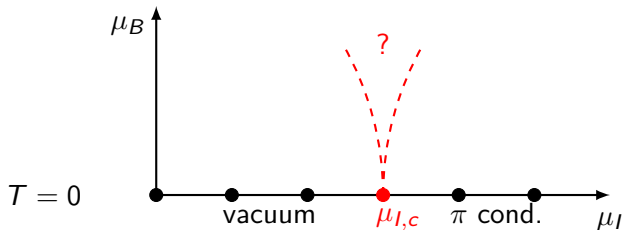


Reweighting in μ : motivation



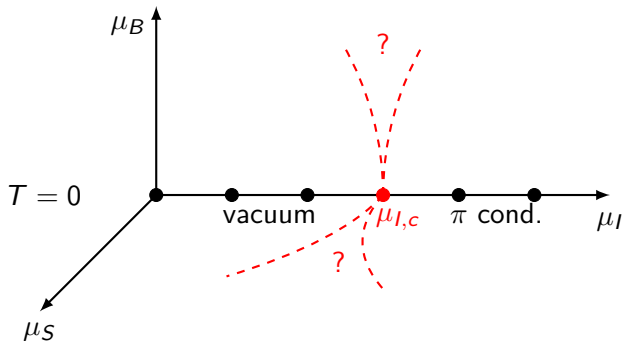
- until now: $\mu_B, \mu_S = 0$

Reweighting in μ : motivation



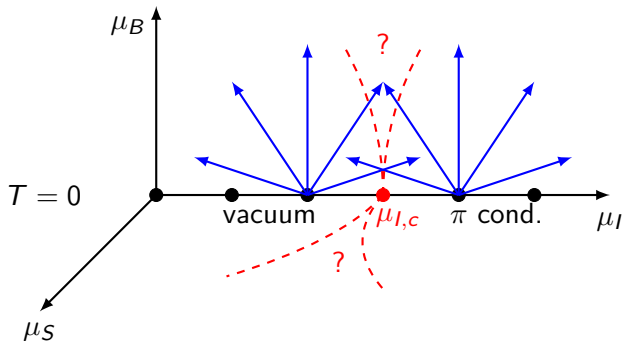
- until now: $\mu_B, \mu_S = 0$
- want to explore $\mu_B > 0$: **phase boundary**

Reweighting in μ : motivation



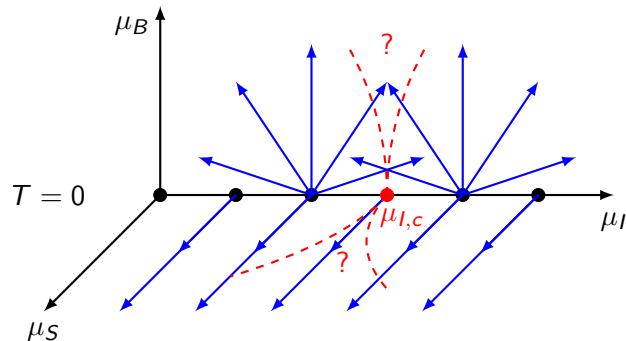
- until now: $\mu_B, \mu_S = 0$
- want to explore $\mu_B > 0, \mu_S > 0$: **phase boundary**

Reweighting in μ : motivation



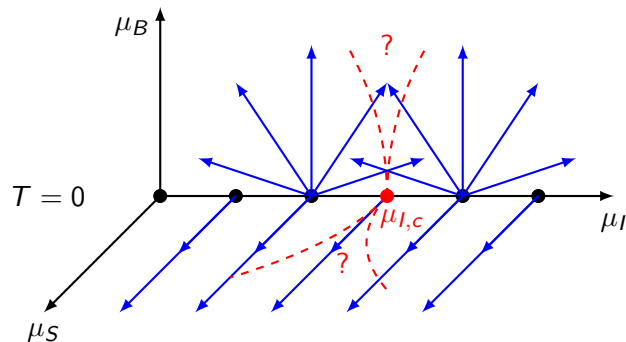
- until now: $\mu_B, \mu_S = 0$
- want to explore $\mu_B > 0, \mu_S > 0$: phase boundary
- reweight from pure μ_I into $\mu_I - \mu_B$ plane

Reweighting in μ : motivation



- until now: $\mu_B, \mu_S = 0$
- want to explore $\mu_B > 0, \mu_S > 0$: **phase boundary**
- **reweight** from pure μ_I into $\mu_I - \mu_B$ and $\mu_I - \mu_S$ plane

Reweighting in μ : motivation



- until now: $\mu_B, \mu_S = 0$
- want to explore $\mu_B > 0, \mu_S > 0$: **phase boundary**
- **reweight** from pure μ_I into $\mu_I - \mu_B$ and $\mu_I - \mu_S$ plane
 - look for lines of constant observables
 - check overlap and sign problem

Reweighting in μ : determinant reduction

- for one quark $R = R_\lambda (\det M_{\mu'} / \det M_\mu)^{1/4}$
- scan over μ_S, μ_B, μ_I : need to compute $\det M_{\mu'}$ for many different μ'

Reweighting in μ : determinant reduction

- for one quark $R = R_\lambda (\det M_{\mu'} / \det M_\mu)^{1/4}$
- scan over μ_S, μ_B, μ_I : need to compute $\det M_{\mu'}$ for many different μ'
- **determinant reduction** [Toussaint '90] [Fodor, Katz '02]

$$\det M_\mu = e^{-3V_s L_t \mu} \det (P - e^{L_t \mu})$$

- **analytic μ -dependence**: calculate eigenvalues of P just once

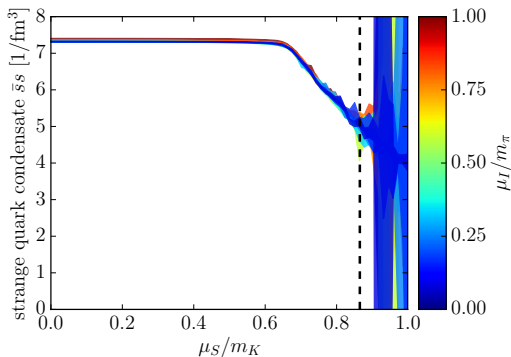
Reweighting in μ : determinant reduction

- for one quark $R = R_\lambda (\det M_{\mu'} / \det M_\mu)^{1/4}$
- scan over μ_S, μ_B, μ_I : need to compute $\det M_{\mu'}$ for many different μ'
- **determinant reduction** [Toussaint '90] [Fodor, Katz '02]

$$\det M_\mu = e^{-3V_s L_t \mu} \det (P - e^{L_t \mu})$$

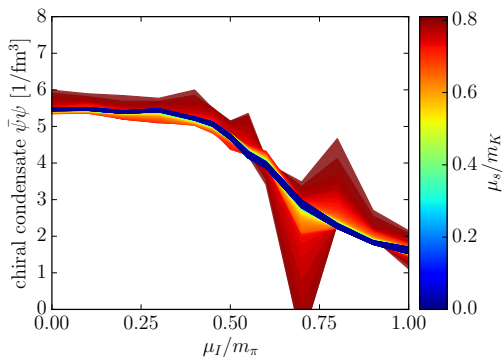
- **analytic μ -dependence**: calculate eigenvalues of P just once
- measure observables in target ensemble
 - $\mu_{u/d} = \mu_B \pm \mu_I$
 - pion condensate $\pi = \frac{T}{V} \frac{\partial \log \mathcal{Z}}{\partial \lambda} \Big|_{\lambda=0}$
 - chiral condensate $\bar{\psi}\psi = \frac{T}{V} \frac{\partial \log \mathcal{Z}}{\partial m_{ud}}$ via numerical derivative
 - benchmark with isospin density $n_I = \frac{T}{V} \frac{\partial \log \mathcal{Z}}{\partial \mu_I}$

Reweighting to $\mu_S > 0$: results



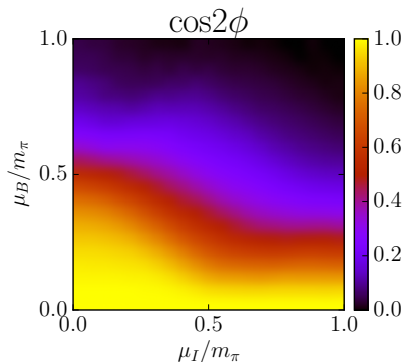
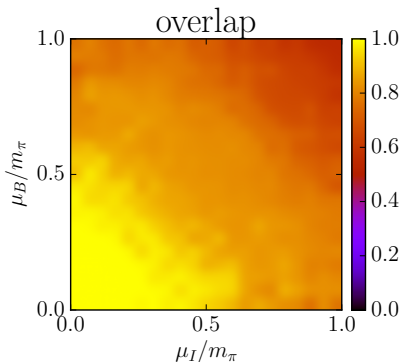
- no kaon cond. below $\mu_S < 0.865 m_K$ [A. Mammarella, M. Mannarelli '15]
- precursor of transition due to finite size / temperature effects

Reweighting to $\mu_S > 0$: results



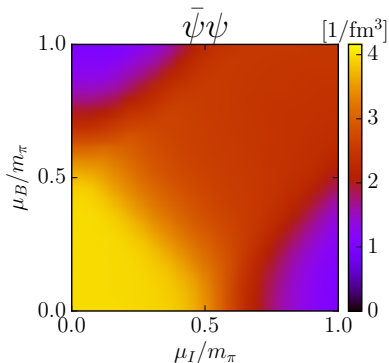
- no kaon cond. below $\mu_S < 0.865 m_K$ [A. Mammarella, M. Mannarelli '15]
- precursor of transition due to finite size / temperature effects
- no visible effect on BEC phase boundary before sign problem gets too strong ($\mu_S \approx 0.7 m_K$)

Reweighting to $\mu_B > 0$: results



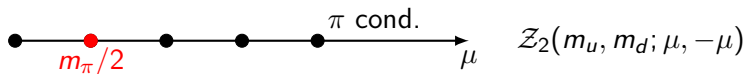
- reasonable overlap, moderate sign problem

Reweighting to $\mu_B > 0$: results



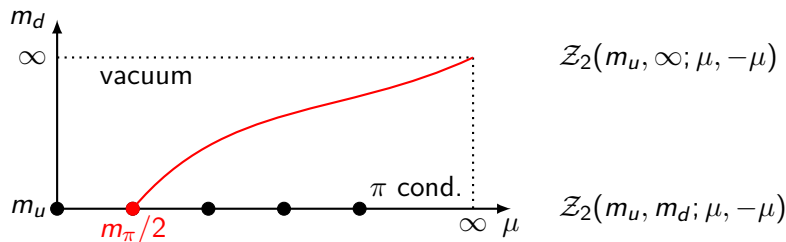
- reasonable overlap, moderate sign problem
- BEC phase boundary bends towards higher values of μ_I
- unexpected behavior below $\mu_{I,c} = m_\pi/2$ (no Silver Blaze for high μ_B)
- strong μ_B -dependence of temperature / finite size effects?

Complementary approach: decouple auxiliary quarks



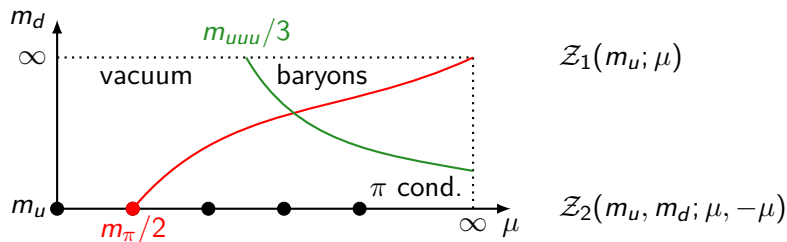
- start from degenerate light quarks with isospin asymmetry

Complementary approach: decouple auxiliary quarks



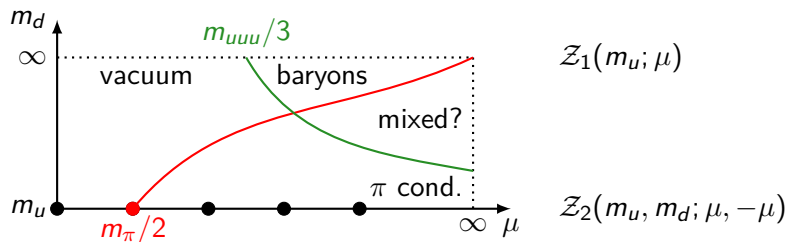
- start from degenerate light quarks with isospin asymmetry
- increase m_d : change in m_π and $\mu_{I,C}$

Complementary approach: decouple auxiliary quarks



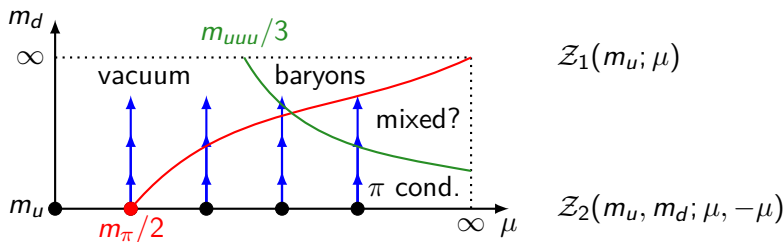
- start from degenerate light quarks with isospin asymmetry
- increase m_d : change in m_π and $\mu_{I,C}$
- $m_d \rightarrow \infty$: **decoupling** of down-quark: **baryonic phase**, **sign problem**

Complementary approach: decouple auxiliary quarks



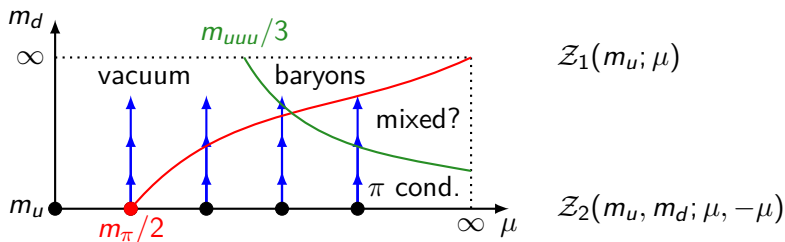
- start from degenerate light quarks with isospin asymmetry
- increase m_d : change in m_π and $\mu_{I,C}$
- $m_d \rightarrow \infty$: **decoupling** of down-quark: **baryonic phase**, **sign problem**

Complementary approach: decouple auxiliary quarks



- start from degenerate light quarks with isospin asymmetry
- increase m_d : change in m_π and $\mu_{I,C}$
- $m_d \rightarrow \infty$: **decoupling** of down-quark: **baryonic phase**, **sign problem**
- via **reweighting** in m_d : $R = R_\lambda [\det(\not{D}_{-\mu} + m_d) / \det(\not{D}_{-\mu} + m_u)]^{1/4}$

Complementary approach: decouple auxiliary quarks



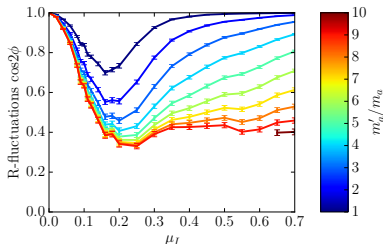
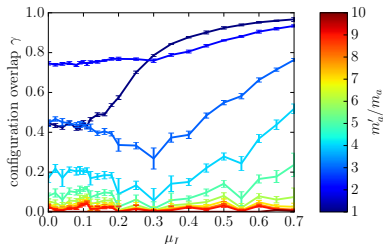
- start from degenerate light quarks with isospin asymmetry
- increase m_d : change in m_π and $\mu_{I,C}$
- $m_d \rightarrow \infty$: **decoupling** of down-quark: **baryonic phase**, **sign problem**
- via **reweighting** in m_d : $R = R_\lambda [\det(\not{D}_{-\mu} + m_d) / \det(\not{D}_{-\mu} + m_u)]^{1/4}$
- want to have $N_f = 2 + 1$ theory after decoupling: start from 5-flavor QCD and repeat above procedure for **2 auxiliary quarks**

Reweighting in m_q : observations

- adding quarks induces drastic changes: different a , m_π , T , $\bar{\psi}\psi$, ... prohibits to formulate clear statement

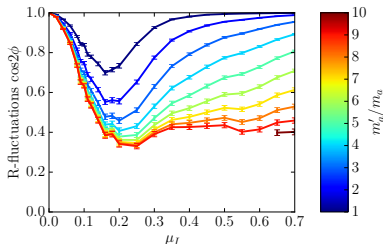
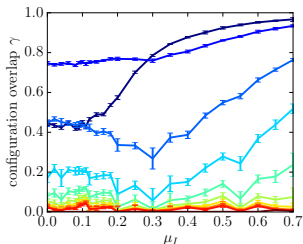
Reweighting in m_q : observations

- adding quarks induces drastic changes: different a , m_π , T , $\bar{\psi}\psi$, ... prohibits to formulate clear statement
- start from higher quark masses to match $\bar{\psi}\psi$ values, lower m_{ud} to physical values together with decoupling auxiliary quarks



Reweighting in m_q : observations

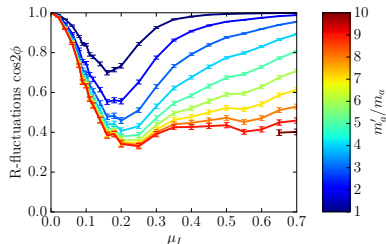
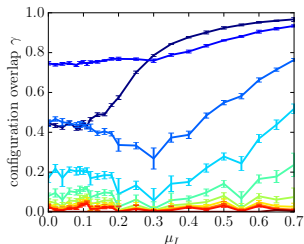
- adding quarks induces drastic changes: different a , m_π , T , $\bar{\psi}\psi$, ... prohibits to formulate clear statement
- start from higher quark masses to match $\bar{\psi}\psi$ values, lower m_{ud} to physical values together with decoupling auxiliary quarks



- see changes in the auxiliary quark sector, but we are more interested in the remaining quarks

Reweighting in m_q : observations

- adding quarks induces drastic changes: different a , m_π , T , $\bar{\psi}\psi$, ... prohibits to formulate clear statement
- start from higher quark masses to match $\bar{\psi}\psi$ values, lower m_{ud} to physical values together with decoupling auxiliary quarks



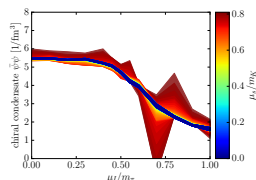
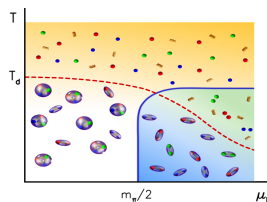
- see changes in the auxiliary quark sector, but we are more interested in the remaining quarks
- optimally: multi-parameter-reweighting in m_a and β

Summary

- QCD with isospin chemical potential
- methods, underlying concepts
- dependence of phase boundary on μ_S, μ_B
- approach via decoupling of quarks

Outlook:

- study temperature / finite size effects



Thank you!

backup: reliability of reweighting

- for normalized $\sum_i R_i = 1$ and sorted $R_1 \geq \dots \geq R_N$, estimate **overlap** γ as [F. Csikor et. al. '04] [C. Schmidt '04]

$$\sum_{i=1}^{N\gamma/2} R_i = 1 - \gamma/2.$$

$$\gamma = \begin{cases} 1 : R_1 = \dots = R_N & \Rightarrow \text{big overlap} \\ 0 : R_1 \gg \sum_{i=2}^N R_i & \Rightarrow \text{only one configuration relevant} \quad \zeta \end{cases}$$

- sign problem**: the phase fluctuation of $R = |R|e^{i\phi}$ is

$$\cos(2\phi) = \Re \frac{R^2}{|R|^2}$$

$$\cos(2\phi) = \begin{cases} 1 : \text{no fluctuations} & \Rightarrow \text{no sign problem} \\ 0 : \text{strong fluctuations} & \Rightarrow \text{severe sign problem} \quad \zeta \end{cases}$$