Exploring the QCD phase diagram via reweighting from isospin chemical potential

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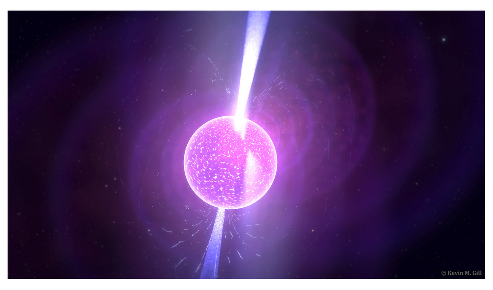
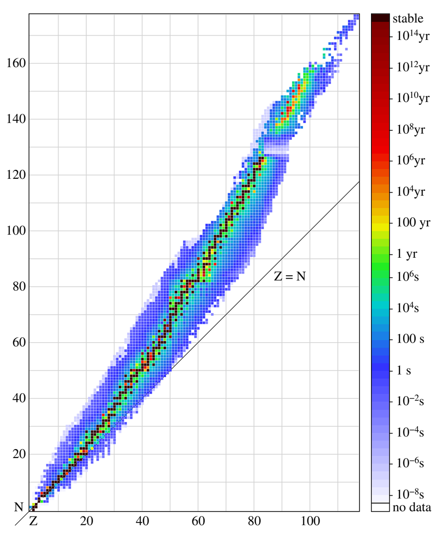
Introduction

Motivation

isospin-asymmetry:
$n_I = n_u - n_d \neq 0$ in

- systems with charged pions
- neutron stars
- heavy-ion collisions (N>Z)



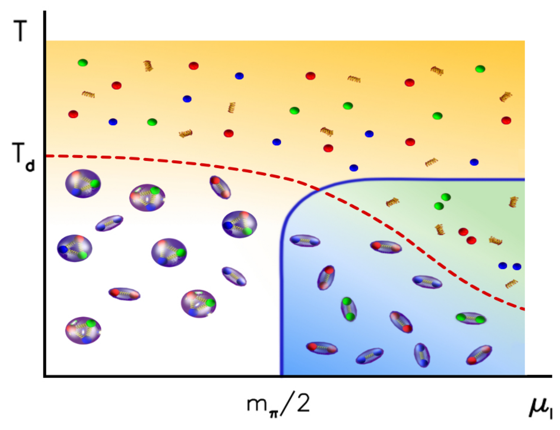


Pure isospin system

rich conjectured phase diagram:

- vacuum (white)
- quark-gluon plasma
- pion condensate (BEC)
- BCS phase

lattice simulations are feasible



Pion condensation: spontaneous symmetry breaking

QCD with two light quarks $\mathcal{M} = \not{D} + m_{ud} + \mu_I \gamma_0 \tau_3 + i\lambda\gamma_5\tau_2$

chiral symmetry breaking pattern $\mathrm{SU}(2)_V \to \mathrm{U}(1)_{\tau_3} \to \varnothing$

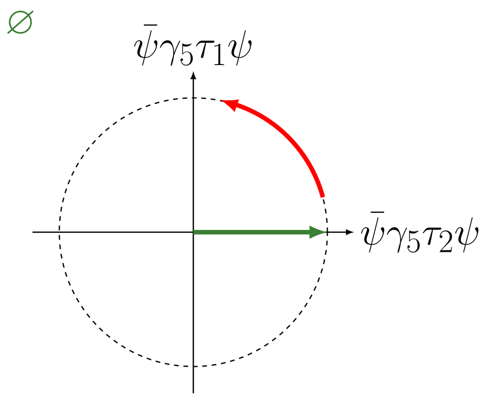
problem: cannot directly observe SSB in finite volumes

- pion condensate $\langle \bar\psi\gamma_5\tau_{1,2}\psi\rangle = 0$ (Goldstone mode)
- accumulation of zero eigenvalues ↯ slowdown of algorithm

solution: add explicit unphysical breaking λ (pionic source)

- can indirectly observe spontaneous symmetry breaking
- no zero eigenvalues

need to **extrapolate $\boldsymbol{\lambda \to 0}$** for physical results



Setup and Observables

Partition function

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

with improved gauge action and staggered quarks at physical masses

$$\mathcal{M}_{ud} = \begin{pmatrix} \not{D}(\mu_I) + m_{ud} & \lambda\eta_5 \\ -\lambda\eta_5 & \not{D}(-\mu_I) + m_{ud} \end{pmatrix}, \quad \mathcal{M}_s = \not{D}(0) + m_s$$

No sign problem: $\mathcal{M}_{ud}$ is $\tau_1\eta_5$-hermitian

Observables

Measures for the BEC phase boundary are pion and chiral condensate, as well as isospin density

$$\langle \pi^{\pm} \rangle_\lambda = \frac{T}{V}\frac{\partial \log \mathcal{Z}_\lambda}{\partial \lambda}, \qquad \langle \bar\psi\psi \rangle_\lambda = \frac{T}{V}\frac{\partial \log \mathcal{Z}_\lambda}{\partial m_{ud}}, \qquad \langle n_I \rangle_\lambda = \frac{T}{V}\frac{\partial \log \mathcal{Z}_\lambda}{\partial \mu_I}.$$

Reweighting in λ

Instead of taking a naive λ-extrapolation $\lim_{\lambda\to 0} \langle O \rangle_\lambda$, we measure the operators O directly at $\lambda = 0$ and reweight the gauge configurations according to

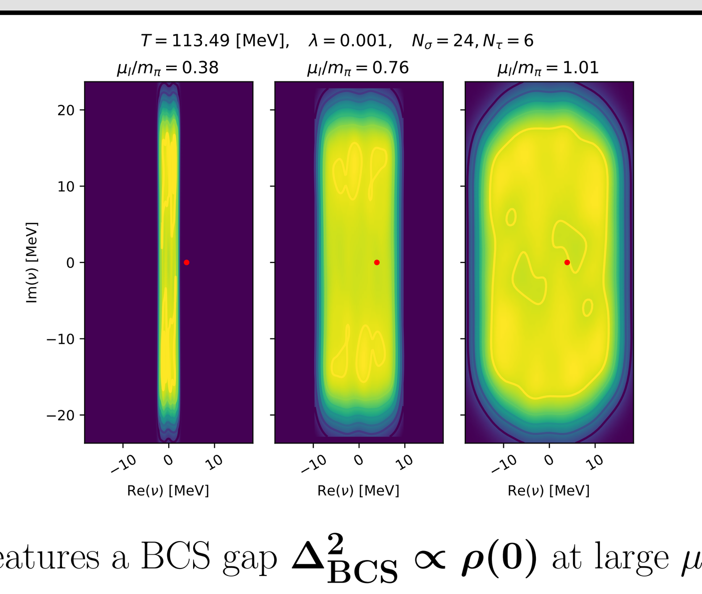
$$\langle O \rangle_0 = \frac{\langle O R_\lambda \rangle_\lambda}{\langle R_\lambda \rangle_\lambda}, \qquad R_\lambda = \left[\frac{\det \mathcal{M}_{ud}(\mu_I, \lambda)}{\det \mathcal{M}_{ud}(\mu_I, 0)}\right]^{1/4} \in \mathbb{R}.$$

Note that measuring the pion condensate at $\lambda = 0$ is only viable via employing a Banks-Casher-type relation similar to [Kanazawa, Wettig, Yamamoto '11]. An **advantage** of reweighting is that it can easily be combined with reweighting in other parameters (e.g μ, m_d, c.f. right column), since $R = R_\lambda R_\mu R_m$. We use leading order reweighting in λ for speedup, without losing accuracy [Brandt, Endrődi, Schmalzbauer '18].

Detection of BCS phase

Status

- We observe large values of the Polyakov loop within the pion condensation phase, which hints to a superconducting ground state with deconfined quarks, the BCS phase
- [Son, Stephanov '01] (χPT) and [Adhikari, Andersen, Kneschke '18] (quark meson model) predict this BEC-BCS crossover to take place at $T = 0$, large μ_I; we see it at $T > 0$ and intermediate μ_I (via Ploop)



- [Kanazawa, Wettig, Yamamoto '14] derive that the BCS phase features a BCS gap $\boldsymbol{\Delta^2_{\mathrm{BCS}} \propto \rho(0)}$ at large μ_I, with $\rho(\nu)$ the density of the complex dirac spectrum
- Motivation to measure $\rho(0)$ as a function of μ_I to identify the BCS phase

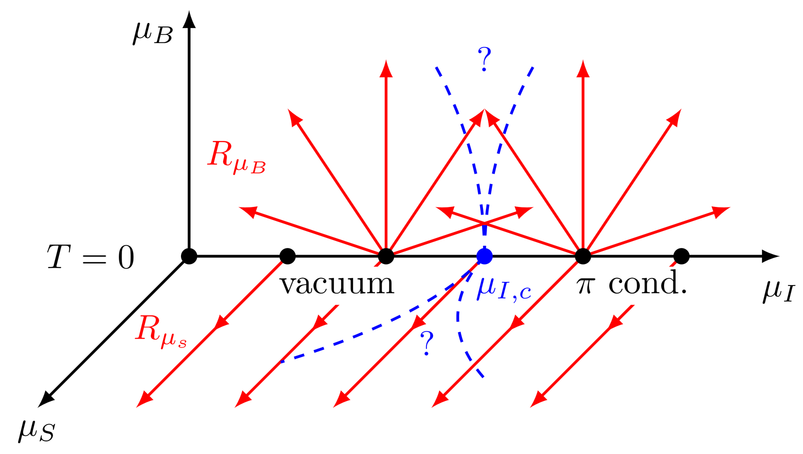
Procedure

- spectrum $\rho(\nu)$ measured close to the origin via SLEPc library employing the Krylov-Schur method
- simulations are carried out away from the chiral limit, investigate $\rho(m + i \cdot 0)$ (denoted by red dot)
- $m + i \cdot 0$ is within the spectrum in the pion condensation phase
- look for sub-structures in the spectral density
- match μ_I- and T- dependence of $\rho(m + i \cdot 0)$ with characteristic points of Polyakov loop
- study $T < 100$ MeV and extrapolate $\lambda \to 0$

Dependence of BEC phase boundary on μ_B, μ_S

Idea

Explore the phase diagram for finite values of $\boldsymbol{\mu_B}$ ($\mu_{u,d} = \mu_B \pm \mu_I$) and $\boldsymbol{\mu_s}$ and study the change in the pion condensation phase boundary, originally at $\mu_{I,c} = m_\pi/2$. The corresponding reweighting factors



$$R_{\mu_B} = \left[\frac{\det \mathcal{M}_{ud}(\mu_u, \mu_d; m_{ud}, m_{ud})}{\det \mathcal{M}_{ud}(\mu_I, -\mu_I; m_{ud}, m_{ud})}\right]^{1/4}$$

$$R_{\mu_s} = \left[\frac{\det \mathcal{M}_s(\mu_s; m_s)}{\det \mathcal{M}_s(0; m_s)}\right]^{1/4}$$

can easily be computed with the determinant reduction formula (see below). We want to distinguish between

- vacuum $\langle \pi \rangle = 0$, $\langle n_I \rangle = 0$, $\langle \bar\psi\psi \rangle = \text{const.}$,
- π cond. $\langle \pi \rangle \neq 0$, $\langle n_I \rangle \neq 0$, $\langle \bar\psi\psi \rangle < \langle \bar\psi\psi \rangle_{\text{vac.}}$

Determinant reduction

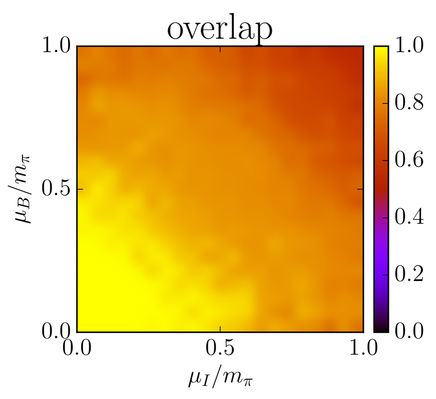
After the λ-reweighting, the fermion determinant factorizes and one can use the **determinant reduction** formula [Toussaint '90][Fodor, Katz '02]

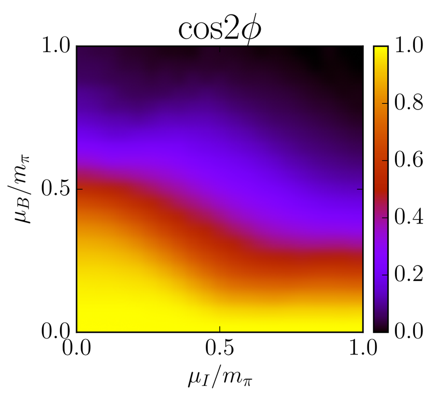
$$\det\left(\not{D}(\mu) + m\right) = e^{-3V_s L_t \mu} \det\left(P(m) - e^{L_t \mu}\right) = e^{-3V_s L_t \mu} \prod_{i=1}^{6V_s} \left(p_i - e^{L_t \mu}\right)$$

to compute the individual terms seperately. Once the matrix $P(m)$ is constructed and its eigenvalues p_i are determined, the fermion determinant is an **analytic function of $\boldsymbol{\mu}$**. Together with the reduction of the dimension of the eigenvalue problem by a factor $N_t/2$, this gives a tremendous boost in terms of computational costs compared to recalculating the full spectrum for each value of μ.

Reliability of reweighting

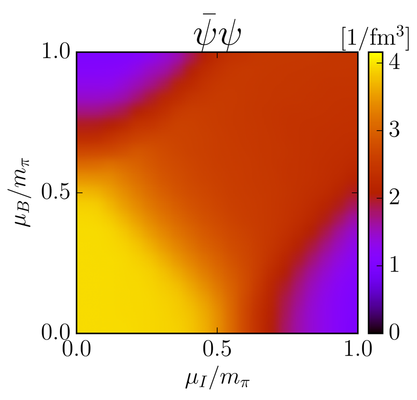
The fluctuations in the phase ϕ of the reweighting factor, which is a measure for the **sign problem**, are only mild close to the isospin axis and for $\mu_B + \mu_I < m_\pi/2$. If the sign problem is severe, one has to be careful whether the results can be trusted. Therefore, we will only show results with **meaningful statists** ($\mathcal{Z} \in \mathbb{R}^+$ within 3σ) and **sufficient overlap $\boldsymbol{\gamma}$** [Csikor et. al. '04] [Schmidt '04].

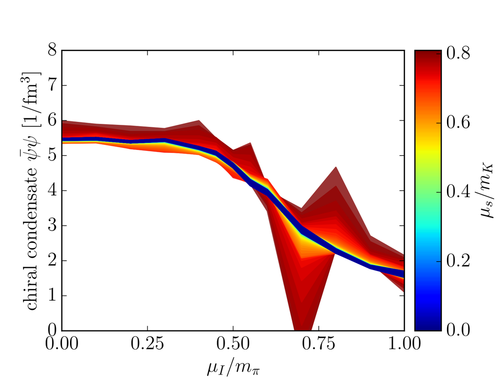




Results

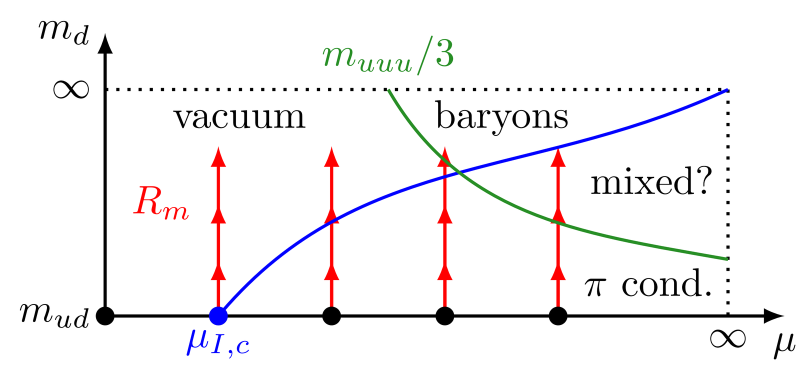
To improve our estimates, we combine multiple auxiliary ensembles. The **BEC phase boundary** bends towards higher values of μ_I for $\mu_B > 0$ and seems to be unaffected by μ_S, before the sign problem gets too severe. We still need to understand the absence of the **silver blaze** phenomenon near the μ_B axis.

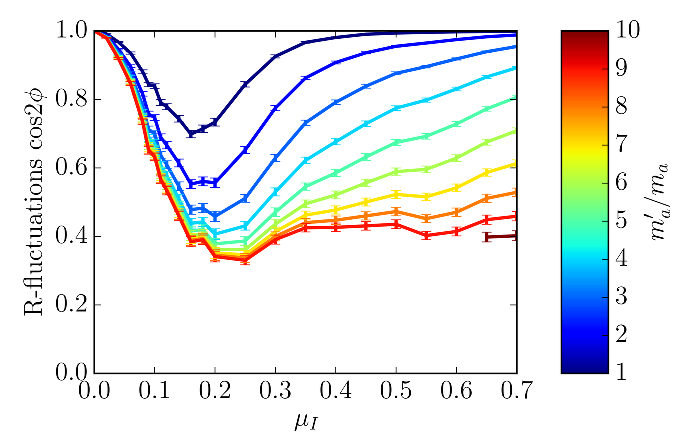




Complementary approach: decoupling of quarks

An additional idea to approach a purely baryonic system is to **decouple one quark** by increasing its mass. Effectively, the isospin system is broken up into a baryonic system, together with the emergence of the sign problem. A sketch of a possible scenario is given below for $\boldsymbol{m_d \to \infty}$. All chemical potentials are held fixed.





Since the quark masses are no longer the same, $m_d > m_u = m_{ud}$, we analyze the quark condensates $\bar u u$, $\bar d d$ separately. Instead of working with a reduced determinant, we compute the full dirac spectrum, since it allows for an analytic m-dependence. To achieve a $N_f = 2 + 1$ target ensemble, we start with two additional auxiliary quarks and decouple those (m_a in right plot). To avoid drastic changes in the system $(a, T, m_\pi, \bar\psi\psi)$, we simulate at higher bare quark mass to account for changes in the lattice scale and LCP. Another possibility would be to adjust β accordingly.