

Phase diagram of isospin-asymmetric QCD: direct results vs Taylor expansion

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in collaboration with

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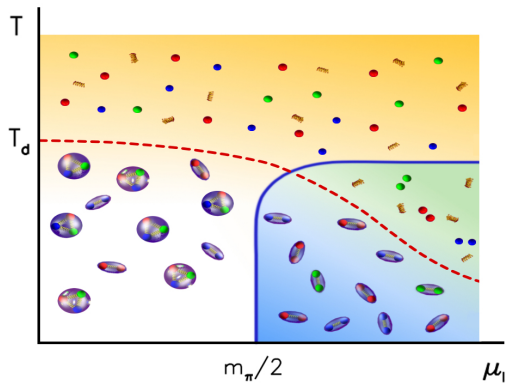


Lattice seminar @ HUB, 26. November 2018

Outline

- introduction: QCD with isospin
 - ▶ pion condensation
 - ▶ spontaneous vs explicit symmetry breaking
- extrapolations in the explicit breaking parameter
 - ▶ singular value representation
 - ▶ leading-order reweighting
 - ▶ Banks-Casher-type improvements
- results
 - ▶ phase diagram
 - ▶ comparison to Taylor expansion
- summary

Main result: phase diagram

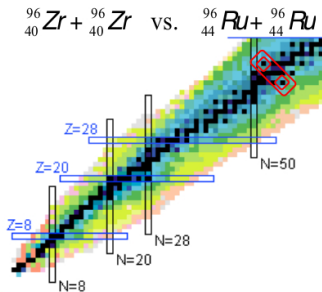


[Brandt, Endrődi, Schmalzbauer 1712.08190]

Introduction

Introduction

- ▶ isospin density $n_I \equiv n_u - n_d$
- ▶ $n_I < 0 \rightarrow$ excess of neutrons over protons
 \rightarrow excess of π^- over π^+
- ▶ why relevant?
 \rightarrow heavy-ion collisions, in particular for isobar runs



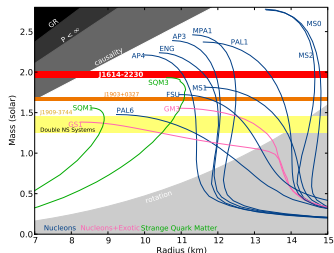
[RHIC isobar program, B. Müller]

Introduction

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- ▶ $n_I < 0 \rightarrow$ excess of neutrons over protons
 \rightarrow excess of π^- over π^+
- ▶ why relevant?
 - \rightarrow heavy-ion collisions, in particular for isobar runs
 - \rightarrow neutron star interiors and composition



[Georgia Tech (Caltech Media Assets)]



[Demorest et al '10]

Isospin chemical potential

- ▶ in the grand canonical ensemble
- ▶ quark chemical potentials (3-flavor)

$$\mu_u = \frac{\mu_B}{3} + \mu_I \quad \mu_d = \frac{\mu_B}{3} - \mu_I \quad \mu_s = \frac{\mu_B}{3} - \mu_S$$

- ▶ zero baryon number, zero strangeness, but **nonzero isospin**

$$\mu_u = \mu_I \quad \mu_d = -\mu_I \quad \mu_s = 0$$

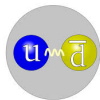
- ▶ pion chemical potential $\mu_\pi = \mu_u - \mu_d = 2\mu_I$



- ▶ isospin density $n_I = n_u - n_d$

Pion condensation

- ▶ QCD at low energies \approx pions
chiral perturbation theory
- ▶ chemical potential for charged pions: μ_π



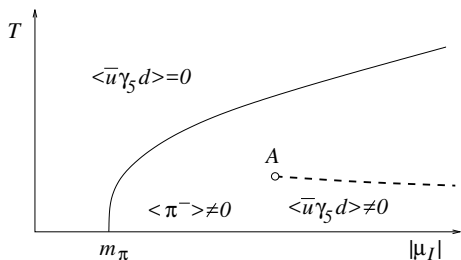
at zero temperature $\mu_\pi < m_\pi$

vacuum state

$\mu_\pi \geq m_\pi$

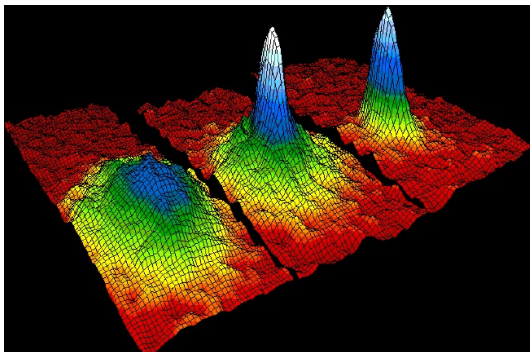
Bose-Einstein condensation

[Son, Stephanov '00]



Bose-Einstein condensate

- ▶ accumulation of bosonic particles in lowest energy state



[Anderson et al '95 JILA-NIST/University of Colorado]

- ▶ velocity distribution of Ru atoms at low temperature
→ peak at zero velocity (zero energy)

BEC in lattice QCD

Symmetry breaking

- ▶ QCD with light quark matrix

$$M = \not{D} + m_{ud}\mathbb{1}$$

- ▶ chiral symmetry (flavor-nontrivial)

$$SU(2)_V$$

Symmetry breaking

- ▶ QCD with light quark matrix

$$M = \not{D} + m_{ud}\mathbb{1} + \mu_1 \gamma_0 \tau_3$$

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

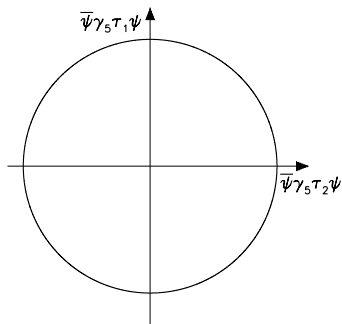
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- ▶ spontaneously broken by a pion condensate

$$\langle \bar{\psi}\gamma_5\tau_{1,2}\psi \rangle$$

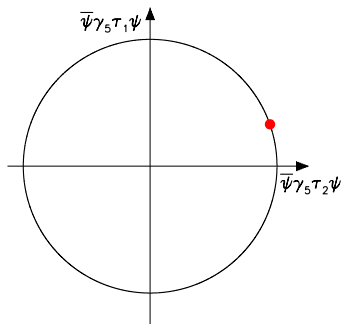
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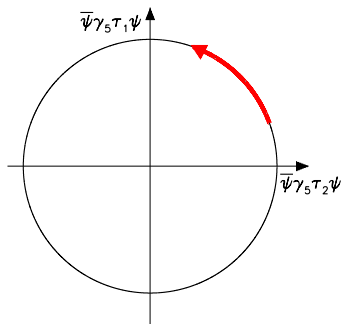
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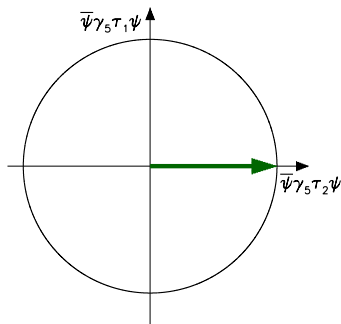
Symmetry breaking

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



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- ▶ a **Goldstone mode** appears
- ▶ add small **explicit breaking**

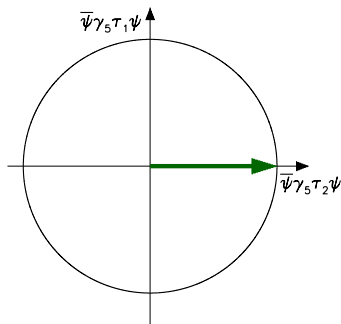
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- ▶ a **Goldstone mode** appears
- ▶ add small **explicit breaking**

- ▶ extrapolate results $\lambda \rightarrow 0$

Dictionary

	pion condensation
pattern	$U(1)_{\tau_3} \rightarrow \emptyset$
coset	$U(1)$
Goldstones	1
spontaneous	$\langle \bar{\psi} \gamma_5 \tau_2 \psi \rangle$
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- ▶ long story short: pion condensation 1/3 as challenging as the chiral limit of the QCD vacuum

Simulation with $\lambda > 0$

- ▶ staggered light quark matrix with $\eta_5 = (-1)^{n_x+n_y+n_z+n_t}$

$$M = \begin{pmatrix} \not{D}_\mu + m & \lambda\eta_5 \\ -\lambda\eta_5 & \not{D}_{-\mu} + m \end{pmatrix}$$

- ▶ we have $\gamma_5\tau_1$ -hermiticity

$$\eta_5\tau_1 M \tau_1 \eta_5 = M^\dagger$$

- ▶ determinant is real and positive

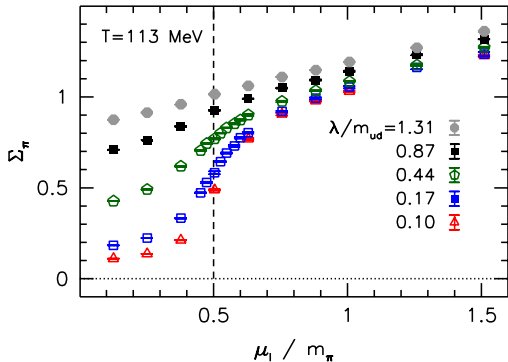
$$\det M = \det(|\not{D}_\mu + m|^2 + \lambda^2)$$

- ▶ early studies [Kogut, Sinclair '02] [de Forcrand, Stephanov, Wenger '07] [Endrődi '14] with unimproved action
- ▶ here: $N_f = 2 + 1$ rooted stout-smearred staggered quarks + tree-level Symanzik improved gluons

Pion condensate on the lattice

- ▶ traditional method [Kogut, Sinclair '02]
measure full operator at nonzero λ (via noisy estimators)

$$\Sigma_\pi \propto \left\langle \text{Tr} M^{-1} \eta_5 \tau_2 \right\rangle$$

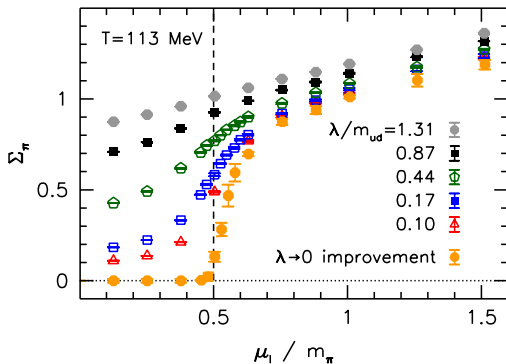


- ▶ extrapolation $\lambda \rightarrow 0$ very steep

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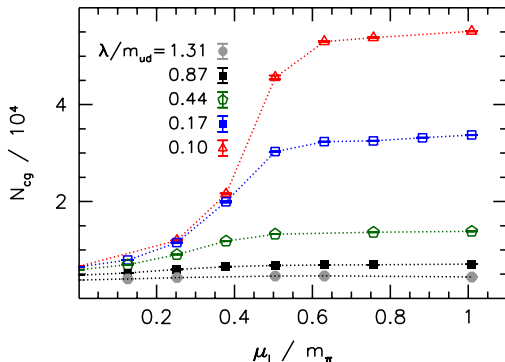
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- ▶ extrapolation $\lambda \rightarrow 0$ very steep
- ▶ new method to extract $\lambda = 0$ limit

Computational cost

- ▶ computational cost for inverting M grows as $\lambda \rightarrow 0$



- ▶ iteration count diverges if a massless mode is present
 \rightsquigarrow alternative definition of pion condensation
- ▶ additionally, reduced step-size necessary due to enhanced fluctuations in fermionic force

Improved λ -extrapolation

Singular value representation

- ▶ singular values

$$|\not{D}_\mu + m|^2 \psi_i = \xi_i^2 \psi_i$$

independent of Dirac eigenvalues due to $[\not{D}_\mu, \not{D}_\mu^\dagger] \neq 0$

- ▶ pion condensate

$$\Sigma_\pi = \frac{\partial}{\partial \lambda} \log \det(|\not{D}_\mu + m|^2 + \lambda^2) = \text{Tr} \frac{2\lambda}{|\not{D}_\mu + m|^2 + \lambda^2}$$

- ▶ spectral representation

$$\Sigma_\pi = \frac{T}{V} \sum_i \frac{2\lambda}{\xi_i^2 + \lambda^2} = \int d\xi \rho(\xi) \frac{2\lambda}{\xi^2 + \lambda^2} \xrightarrow{\lambda \rightarrow 0} \pi \rho(0)$$

first derived in [Kanazawa, Wettig, Yamamoto '11]

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- ▶ compare to Banks-Casher-relation at $\mu_I = 0$

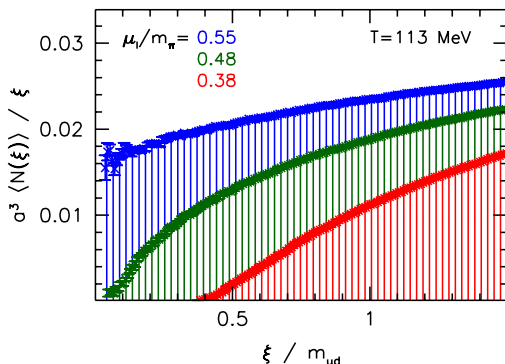
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coset	$U(1)$	$SU(2)_A$
Goldstones	1	3
spontaneous	$\langle \bar{\psi} \gamma_5 \tau_2 \psi \rangle$	$\langle \bar{\psi} \psi \rangle$
explicit	$\lambda \rightarrow 0$	$m \rightarrow 0$
Banks-Casher	$\rho \not{D}_\mu + m ^2(0)$	$\rho \not{D}(0)$

Singular value density

- integrated spectral density

$$N(\xi) = \int_0^\xi d\xi' \rho(\xi'), \quad \rho(0) = \lim_{\xi \rightarrow 0} N(\xi)/\xi$$

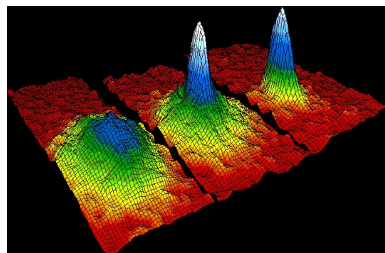
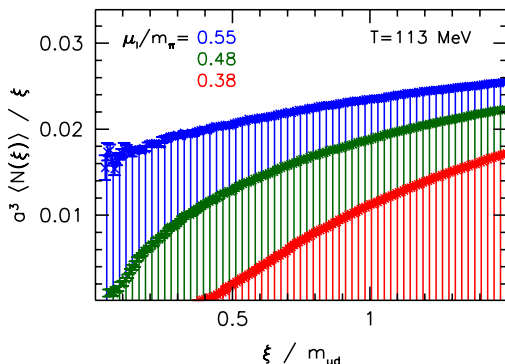


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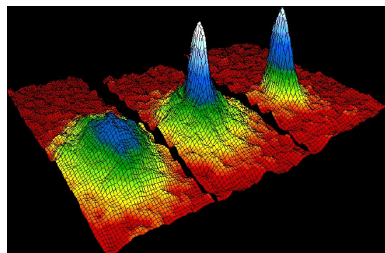
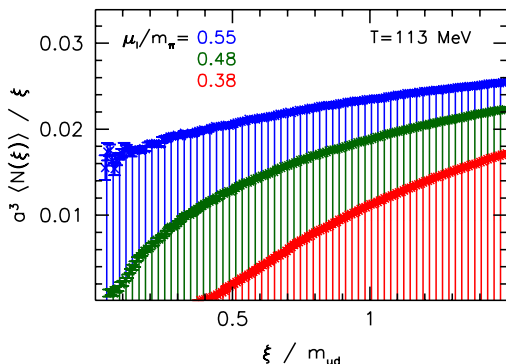
- ▶ compare $\rho(0)$ to velocity distribution around zero

Singular value density

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- ▶ compare $\rho(0)$ to velocity distribution around zero
- ▶ Bose-Einstein condensation!

Reweighting

- ▶ reweighting factor

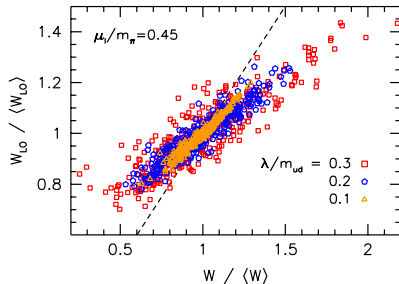
$$W = \frac{\det(|\not{D}_\mu + m|^2)}{\det(|\not{D}_\mu + m|^2 + \lambda^2)}$$

- ▶ but λ is small, so expand in it:

$$W_{\text{LO}} = \exp[-\lambda V_4 \cdot \Sigma_\pi]$$

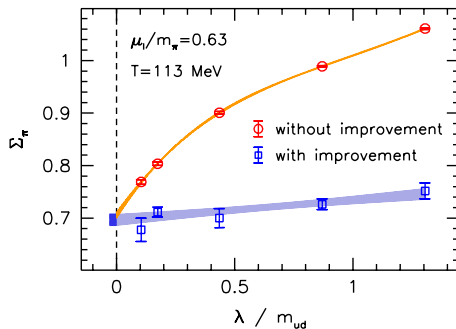
$$\langle \mathcal{O} \rangle_{\text{rew}} = \frac{\langle \mathcal{O} W_{\text{LO}} \rangle}{\langle W_{\text{LO}} \rangle} + \text{higher orders in } \lambda$$

- ▶ scatter plot: W_{LO} vs. W on small lattices



Comparison between old and new methods

- ▶ improvement is crucial for reliable $\lambda \rightarrow 0$ extrapolation

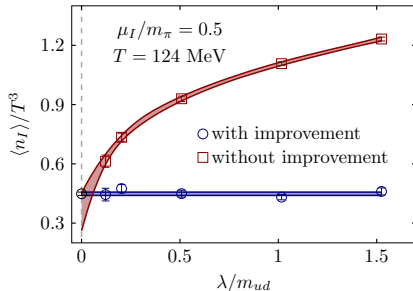
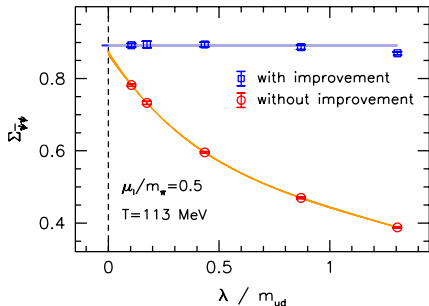


New method for other observables

- ▶ spectral representation for quark condensate

$$\bar{\psi}\psi = \frac{2T}{V} \sum_i \text{Re} \frac{\langle \psi_i | (\not{D}_\mu + m)^\dagger | \psi_i \rangle}{\xi_i^2 + \lambda^2}$$

$$n_I = \frac{2T}{V} \sum_i \text{Re} \frac{\langle \psi_i | (\not{D}_\mu + m)^\dagger \not{D}'_\mu | \psi_i \rangle}{\xi_i^2 + \lambda^2}$$

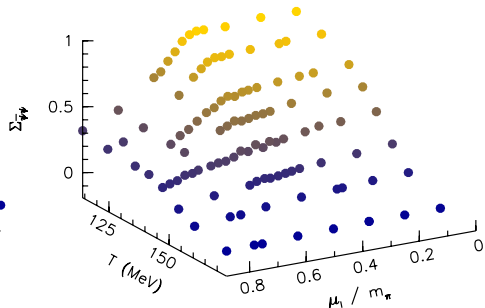
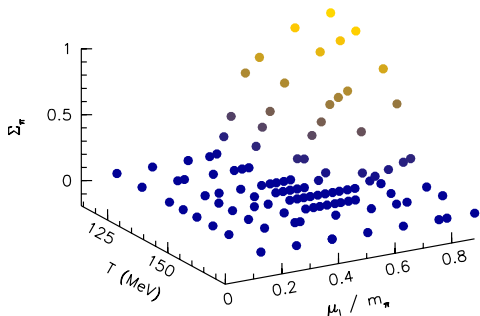


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Results: phase diagram [1712.08190]

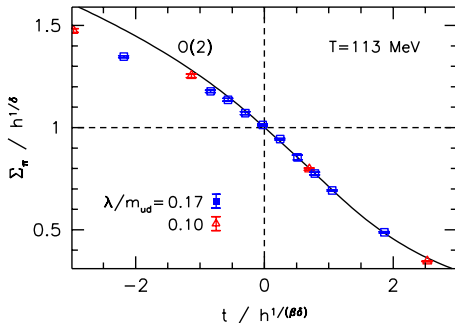
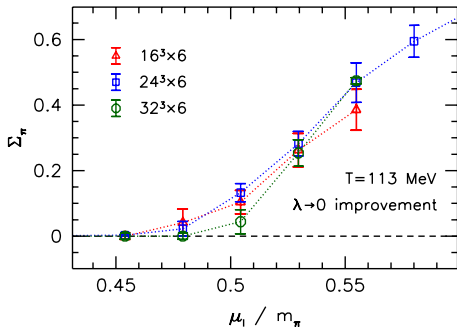
Condensates

- ▶ pion and chiral condensate after $\lambda \rightarrow 0$ extrapolation



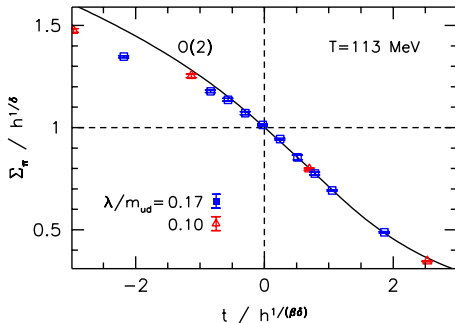
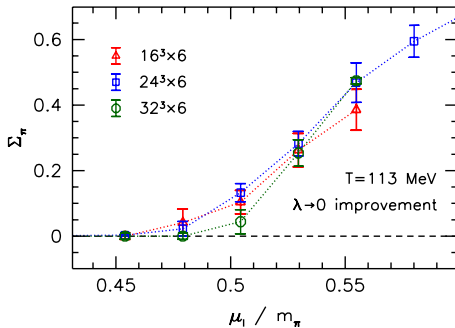
- ▶ read off chiral crossover $T_{pc}(\mu_I)$ and pion condensation boundary $\mu_{I,c}(T)$

Order of the transition



- ▶ volume scaling of order parameter shows typical sharpening
- ▶ collapse according to O(2) critical exponents [Ejiri et al '09]

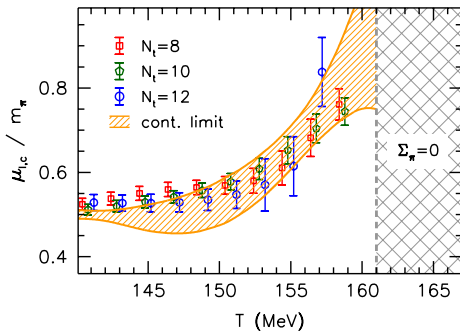
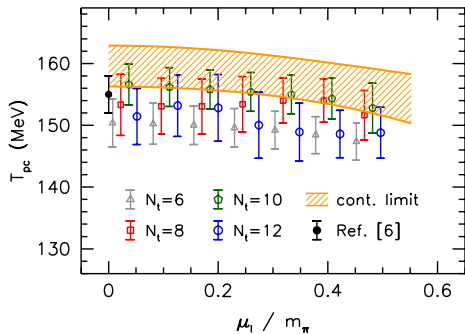
Order of the transition



- ▶ volume scaling of order parameter shows typical sharpening
- ▶ collapse according to $O(2)$ critical exponents [Ejiri et al '09]
- ▶ indications for a second order phase transition at $\mu_I \approx m_\pi/2$, in the $O(2)$ universality class

Transition temperatures

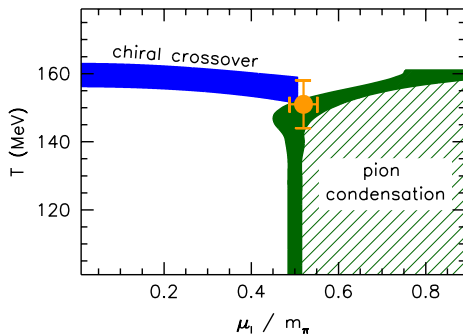
- ▶ T_{pc} : inflection point of chiral condensate
- ▶ $\mu_{I,c}$: boundary of $\Sigma_\pi > 0$ region
- ▶ continuum limit based on $N_t = 6, 8, 10, 12$



Phase diagram

- ▶ meeting point of chiral crossover and pion condensation boundary: *pseudo-triple point*

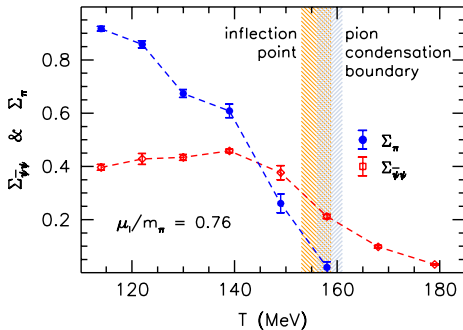
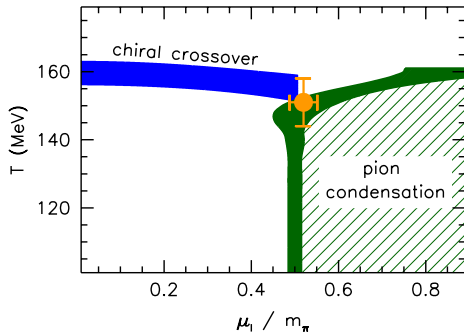
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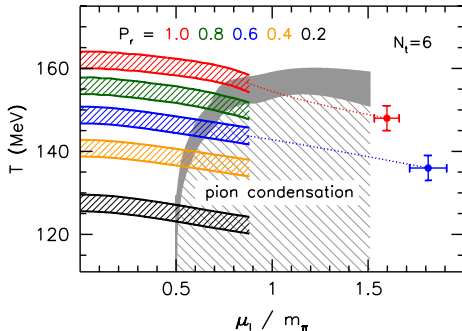
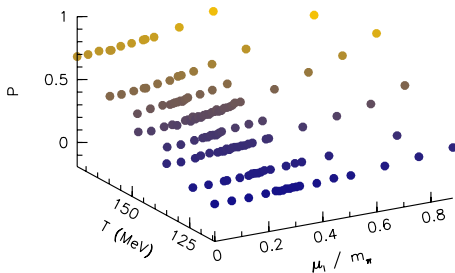
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- ▶ the two transitions coincide beyond the pseudo-triple point

Phase diagram

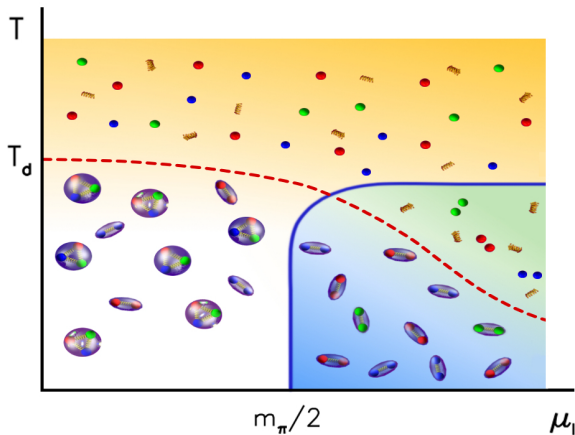
- ▶ Polyakov loop as measure for deconfinement



- ▶ no significant response in P on pion condensation
- ▶ deconfinement crossover persists in pion condensed phase
 \rightsquigarrow BCS superconductivity [Son, Stephanov '01]

Phase diagram

- ▶ favored phase diagram schematically:
hadronic, quark-gluon plasma, BEC, BCS phases



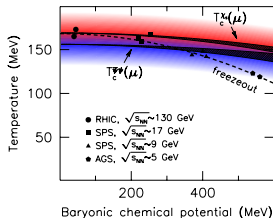
Taylor expansion method

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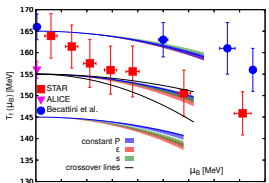
- ▶ overcome sign problem at $\mu_B > 0$
- ▶ reconstruct observable $\mathcal{O}(\mu_B)$ via

$$\mathcal{O}(\mu_B) = \sum_{i=0}^{\infty} c_i^{\mathcal{O}} \mu_B^i$$

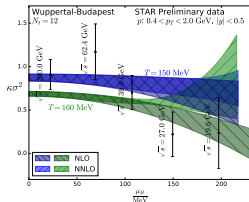
- ▶ routinely used for phase diagram and for EoS



[Endrődi et al '11]



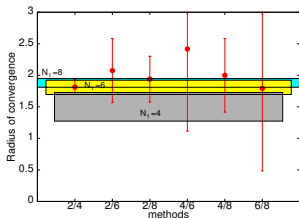
[HotQCD '17]



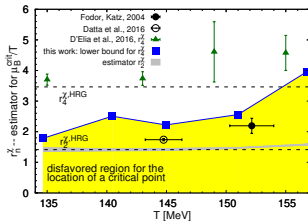
[BMWc '18]

Radius of convergence

- ▶ reconstruction via Taylor expansion only works for analytic functions
- ▶ radius of convergence marks nearest singularity
- ▶ used to investigate the QCD critical endpoint



[Datta, Gavai, Gupta '17]



[HotQCD '17]

Taylor expansion for nonzero isospin

- ▶ comparison between full results and expansion is possible
- ▶ our choice for the observable:

$$\langle n_I \rangle = \frac{T}{V} \frac{\partial \log \mathcal{Z}}{\partial \mu_I}$$

- ▶ compared to Taylor-expansion

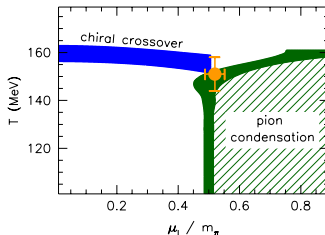
$$\frac{\langle n_I \rangle}{T^3} = \langle c_2 \rangle \cdot \frac{\mu_I}{T} + \frac{\langle c_4 \rangle}{6} \cdot \left(\frac{\mu_I}{T} \right)^3 + \mathcal{O}(\mu_I^5)$$

with $\langle c_{2,4} \rangle$ available in [\[Borsányi et al '12\]](#)

Results: comparison to Taylor series [1810.11045]

Breakdown at pion condensation onset

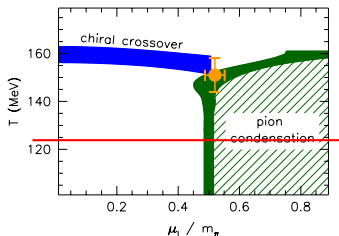
- ▶ second-order phase transition along condensation onset



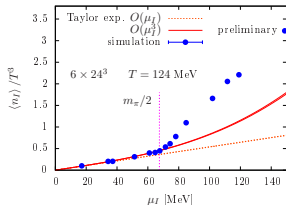
- ▶ Taylor expansion breaks down at the phase transition visualized for the $24^3 \times 6$ ensemble

Breakdown at pion condensation onset

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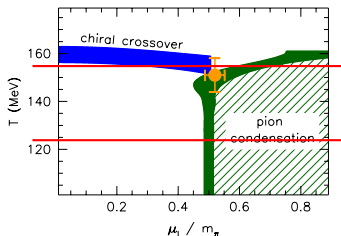


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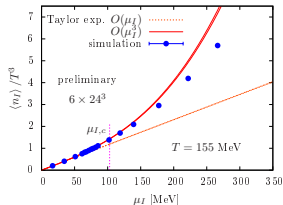
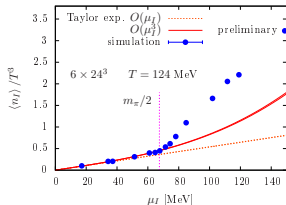


Breakdown at pion condensation onset

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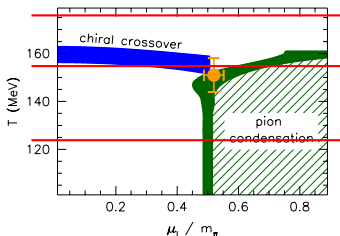


- ▶ Taylor expansion breaks down at the phase transition visualized for the $24^3 \times 6$ ensemble

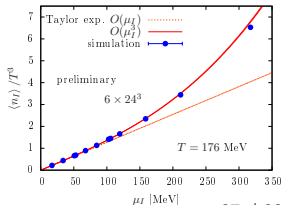
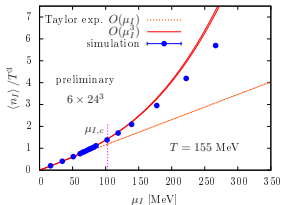
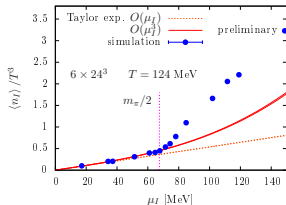


Breakdown at pion condensation onset

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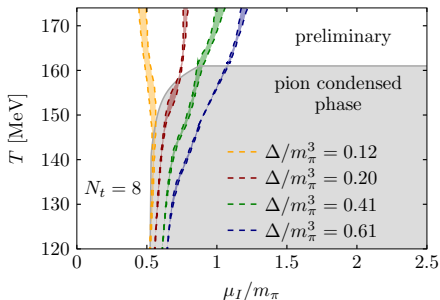
Reliability range

- ▶ quantify deviation between expanded and true values

$$\Delta^{\text{LO}} = \left| \frac{\langle n_I \rangle}{T^3} - \langle c_2 \rangle \cdot \frac{\mu_I}{T} \right| \quad \Delta^{\text{NLO}} = \left| \frac{\langle n_I \rangle}{T^3} - \langle c_2 \rangle \cdot \frac{\mu_I}{T} - \frac{\langle c_4 \rangle}{6} \cdot \left(\frac{\mu_I}{T} \right)^3 \right|$$

- ▶ different behavior inside and outside pion condensed phase

leading order



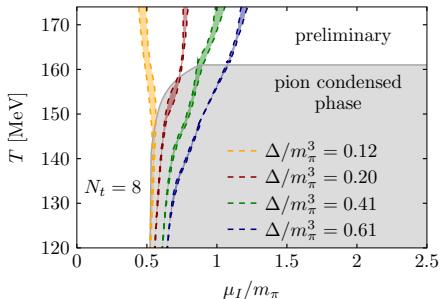
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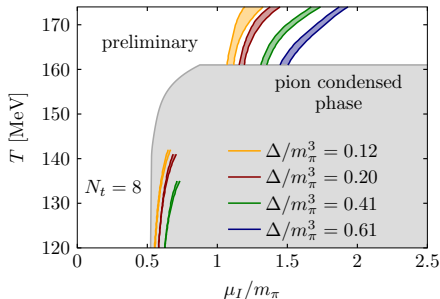
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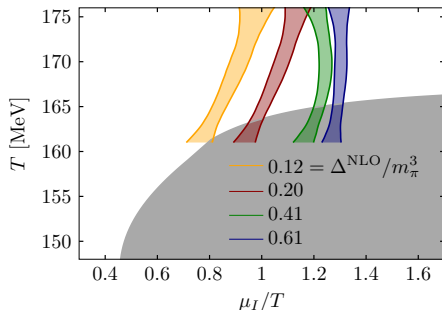


next-to-leading order



Contour lines in the continuum

- ▶ continuum extrapolation performed using $N_t = 6, 8, 10, 12$
- ▶ plot contours against μ_I/T



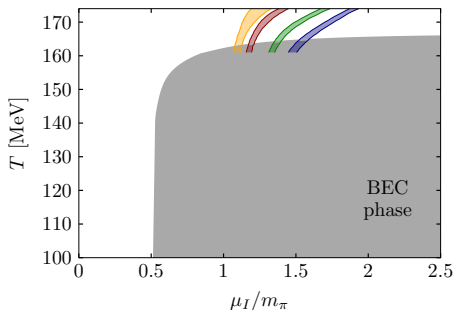
- ▶ large deviations from naively expected $\mu_I/T = \text{const}$ lines

Radius of convergence

- ▶ at low T , nearest singularity is at pion condensation onset
- ▶ radius of convergence for $\chi_I = \partial n_I / \partial \mu_I$:

$$\frac{r}{T} = \lim_{n \rightarrow \infty} \sqrt{\frac{\langle c_n \rangle}{\langle c_{n+2} \rangle} \cdot (n-1)n} \sim \sqrt{\frac{\langle c_2 \rangle}{\langle c_4 \rangle}} \cdot 2$$

using $\langle c_{2,4} \rangle$ from [Borsányi et al '12]

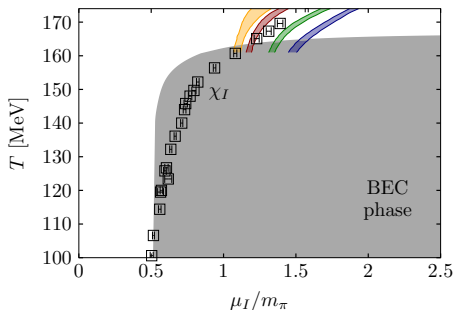


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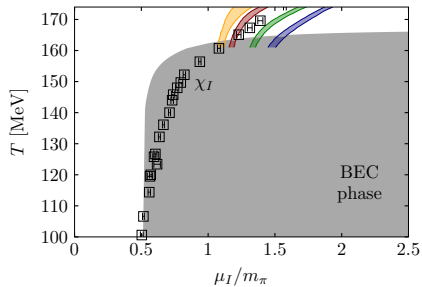
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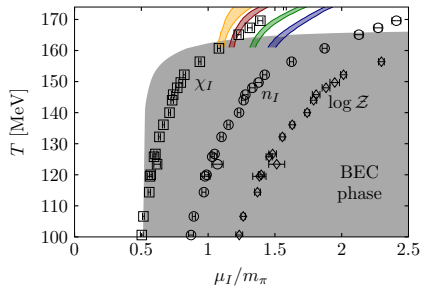
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Estimator from which series?

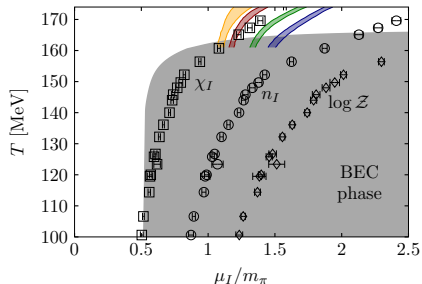


Estimator from which series?



- ▶ $r\{n'_I\} = r\{n_I\} = r\{\log Z\}$, but leading estimators differ as
1 : $\sqrt{3}$: $\sqrt{6}$

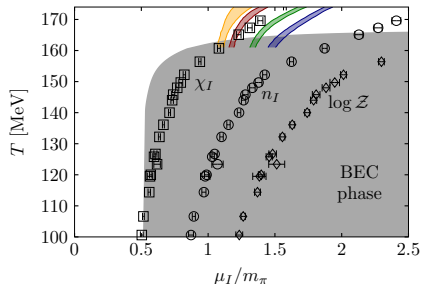
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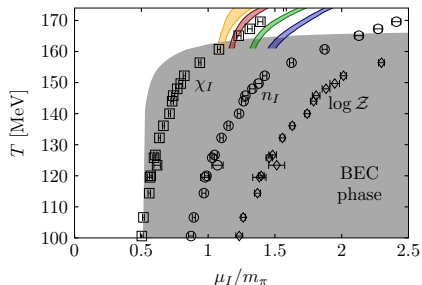
susceptibility-series seems to converge faster
(see also [Karsch, Schaefer, Wagner, Wambach '11])

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- ▶ need higher-order estimates
- ▶ results may give insight to convergence properties at $\mu_B > 0$

Summary

- ▶ Bose-Einstein condensation via singular value density
 \rightsquigarrow flat extrapolation in λ
- ▶ map QCD phase diagram for nonzero isospin-asymmetry
 \rightsquigarrow detected a 2nd order phase transition in full QCD (for the first time)
- ▶ comparison to Taylor expansion around $\mu_I = 0$
 \rightsquigarrow susceptibility series optimal for convergence radius studies

