Reliability of Taylor-expansions in QCD

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in collaboration with
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Outline

- introduction: Taylor expansion
- introduction: isospin chemical potentials
- auxiliary pion source λ
  - inclusion in the action
  - $\lambda \to 0$ extrapolation for physical results
  - singular value representation
- comparison between full results and expansion
  - breakdown of Taylor-method at the phase transition
  - reliability of LO and NLO expansions
- summary

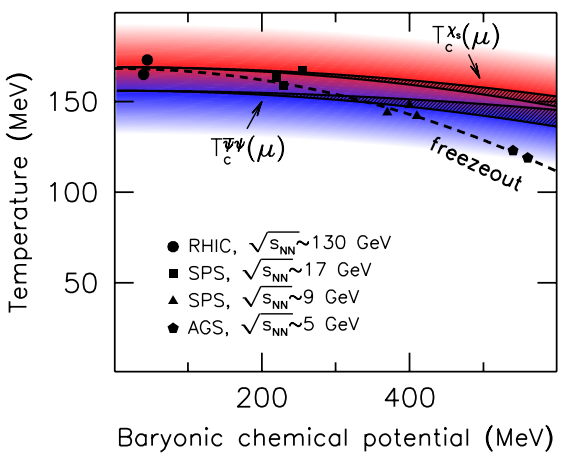
Introduction

Taylor expansion method

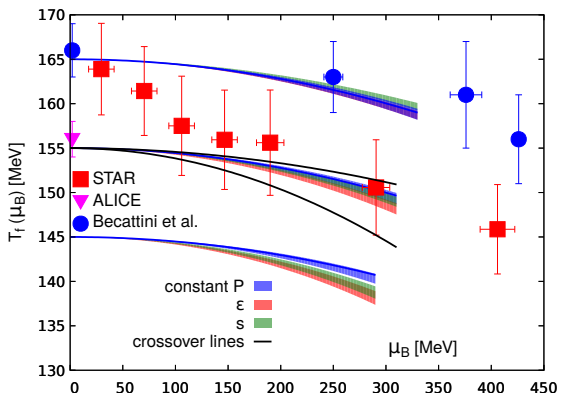
- overcome sign problem at $\mu_B > 0$
- reconstruct observable $\mathcal{O}(\mu_B)$ via

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

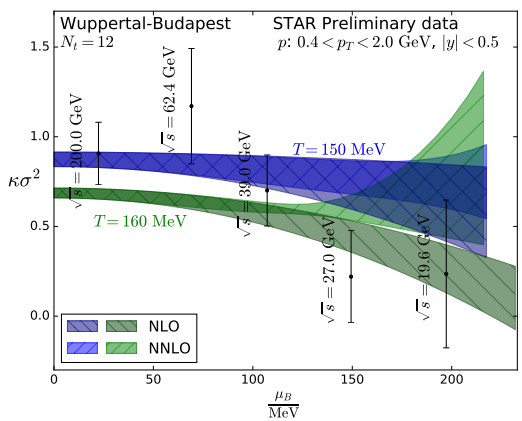
- routinely used for phase diagram and for EoS



[Endrődi et al '11]



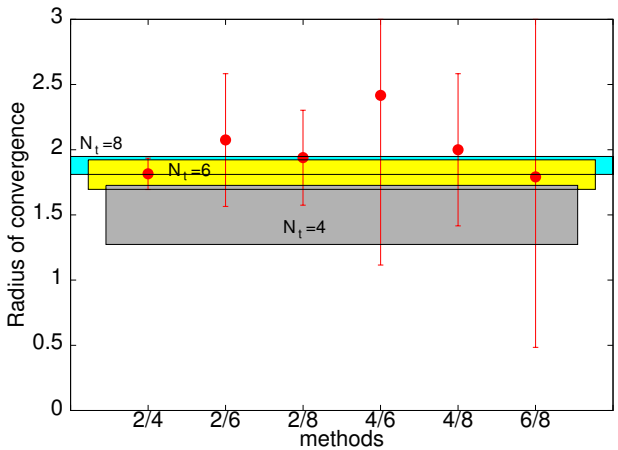
[HotQCD '17]



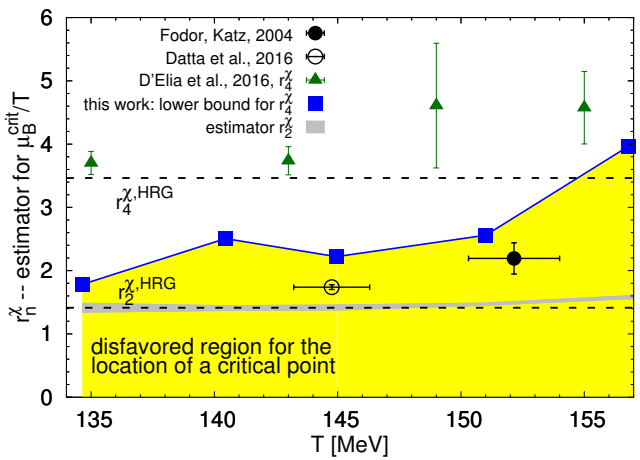
[BMWc '18]

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]

QCD at nonzero isospin

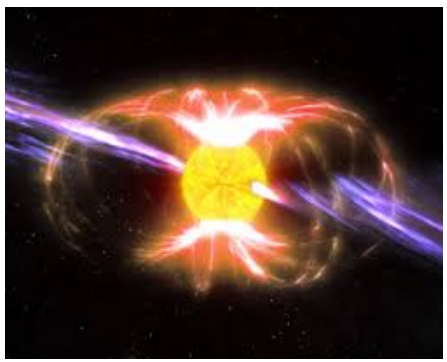
- QCD with zero baryon $\mu_B = 0$

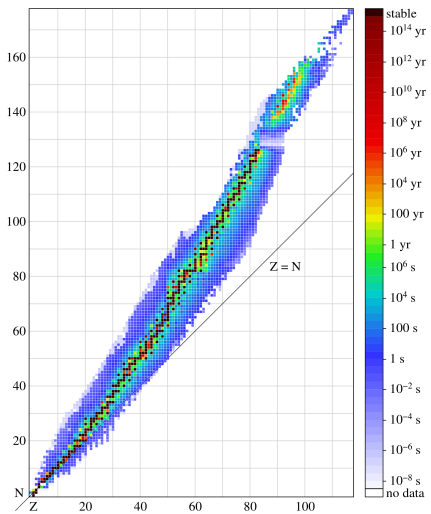
  but nonzero isospin chemical potential $\mu_I \neq 0$

  $\mu_u = \mu_I, \;\; \mu_d = -\mu_I, \;\; \mu_s = 0$

- free of the sign problem
- isospin density $n_I = n_u - n_d$
- $n_I < 0 \rightarrow$ excess of neutrons over protons
  $\rightarrow$ excess of π^- over π^+

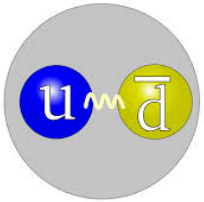
- applications
  - neutron stars
  - heavy-ion collisions





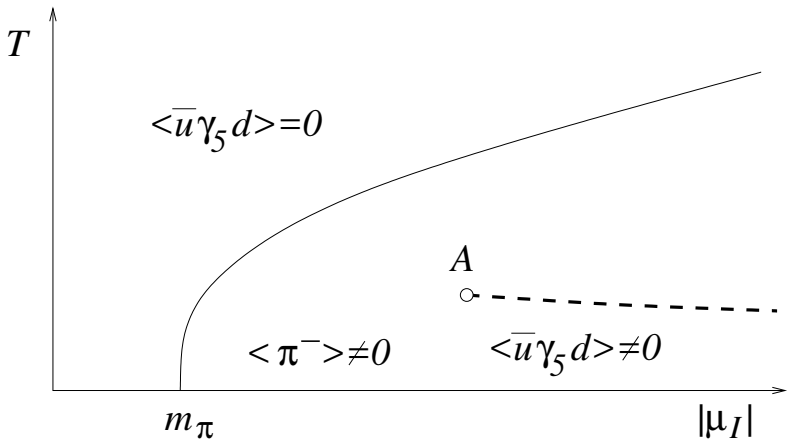
Phase diagram for nonzero isospin

- QCD at low energies $\approx$ pions
  chiral perturbation theory
- chemical potential for charged pions: $\mu_\pi = 2\mu_I$

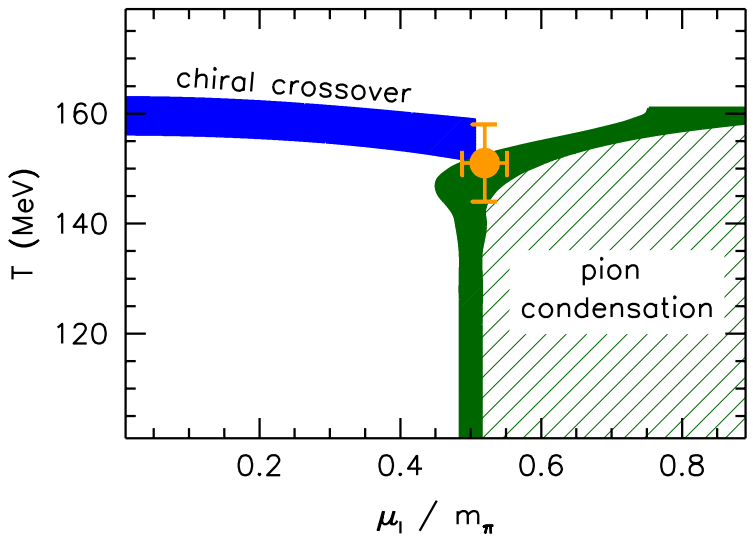


at zero temperature $\mu_\pi < m_\pi$ vacuum state

$\mu_\pi \geq m_\pi$ Bose-Einstein condensation



[Son, Stephanov '00]



[Brandt, Endrődi, Schmalzbauer '18]

Setup

Symmetry breaking

- QCD with light quark matrix

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

- chiral symmetry (flavor-nontrivial)

$$\mathrm{SU}(2)_V$$

Symmetry breaking

- QCD with light quark matrix

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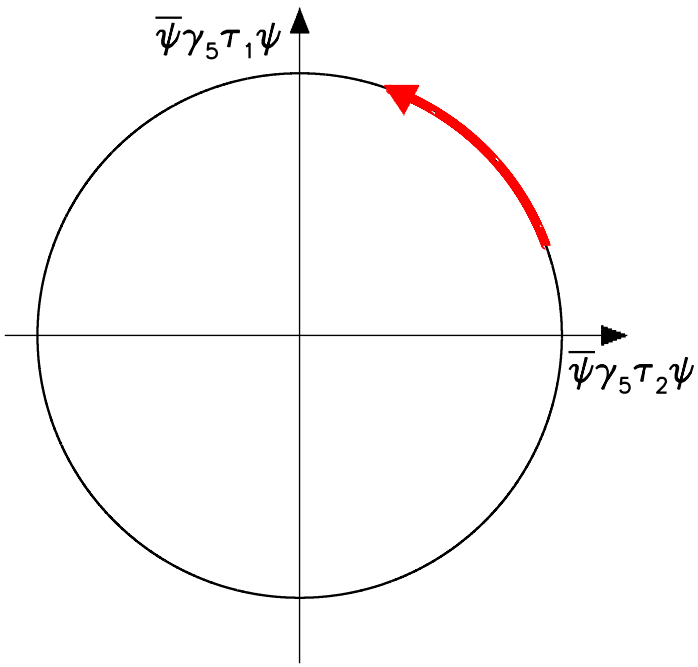

- spontaneously broken by a pion condensate

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

- a Goldstone mode appears

Symmetry breaking

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$$M = \not{D} + m_{ud}\mathbb{1} + \mu_I \gamma_0 \tau_3 + i\lambda\gamma_5\tau_2$$

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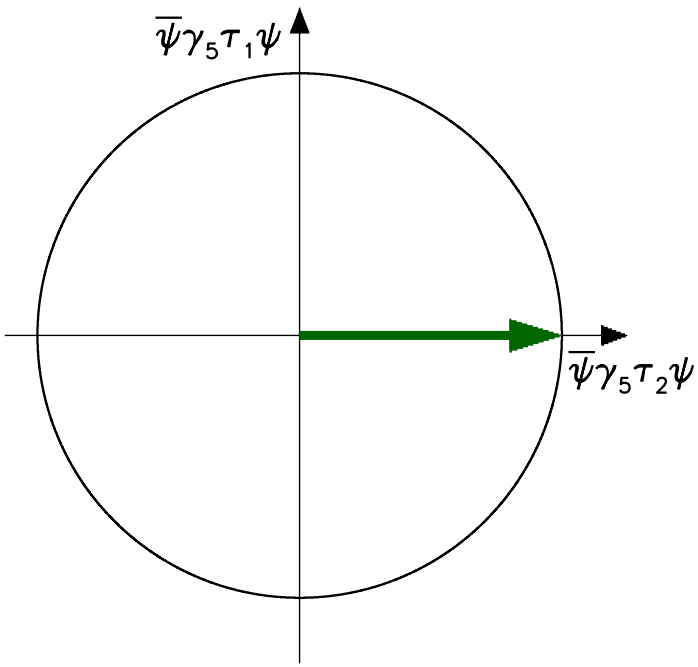

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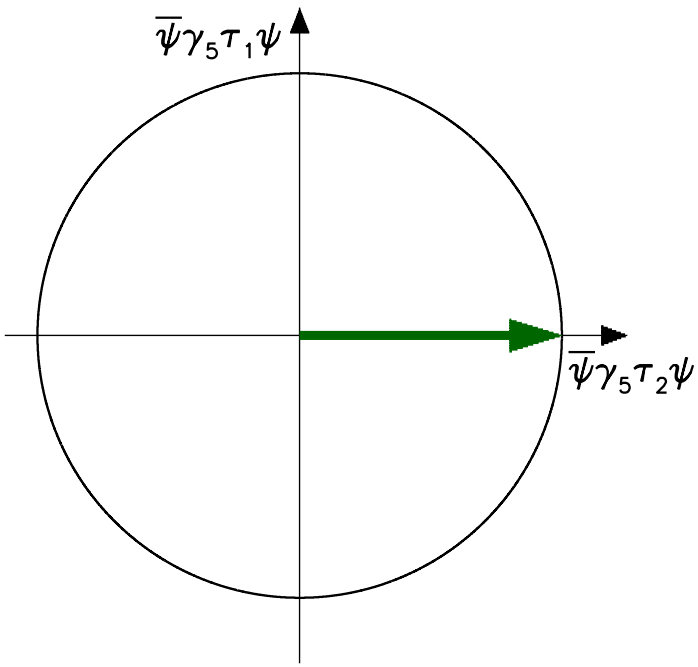

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- extrapolate results $\lambda \to 0$

Simulation details

- 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

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

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

Isospin density

- 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]

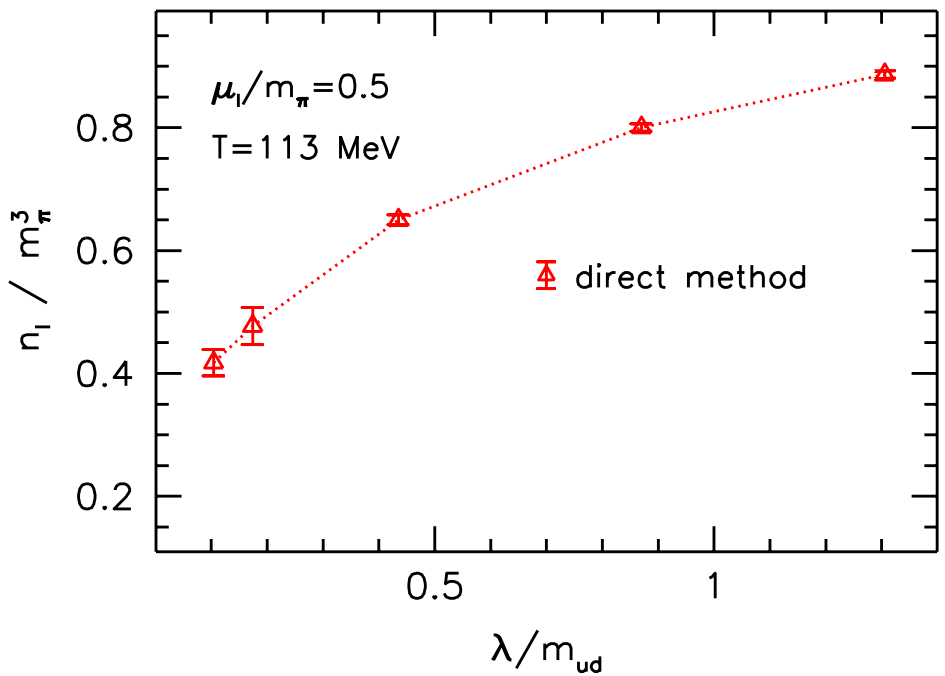
- need $\lambda \to 0$ limit of $\langle n_I \rangle$ for meaningful comparison

$\lambda \to 0$ extrapolation

Need for improvement

- direct method: very large λ-artefacts

$$\langle n_l(\lambda) \rangle_\lambda$$



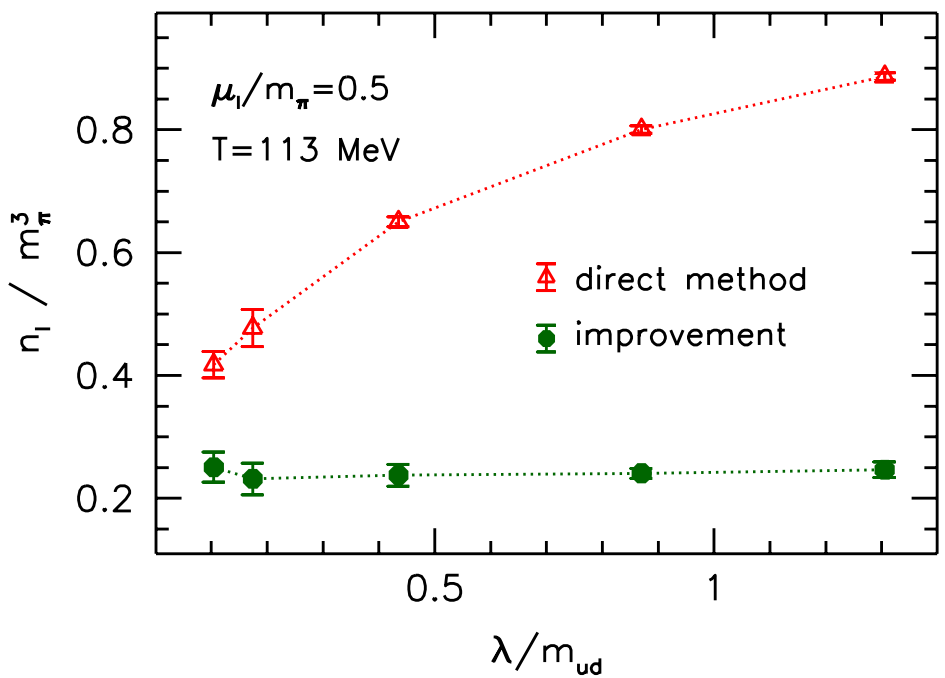
Need for improvement

- direct method: very large λ-artefacts

$$\langle n_I(\lambda) \rangle_\lambda$$

- improvement program: artefacts eliminated

$$\langle n_I(0) \rangle_0$$



Singular value representation

- isospin density

$$n_I = \frac{T}{V}\frac{\partial}{\partial \mu_I}\log\det(|\not{D}_\mu + m|^2+\lambda^2) = \frac{2T}{V}\,\mathrm{Re}\,\mathrm{Tr}\frac{(\not{D}_\mu + m)^\dagger \not{D}'_\mu}{|\not{D}_\mu + m|^2 + \lambda^2}$$

- singular values

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

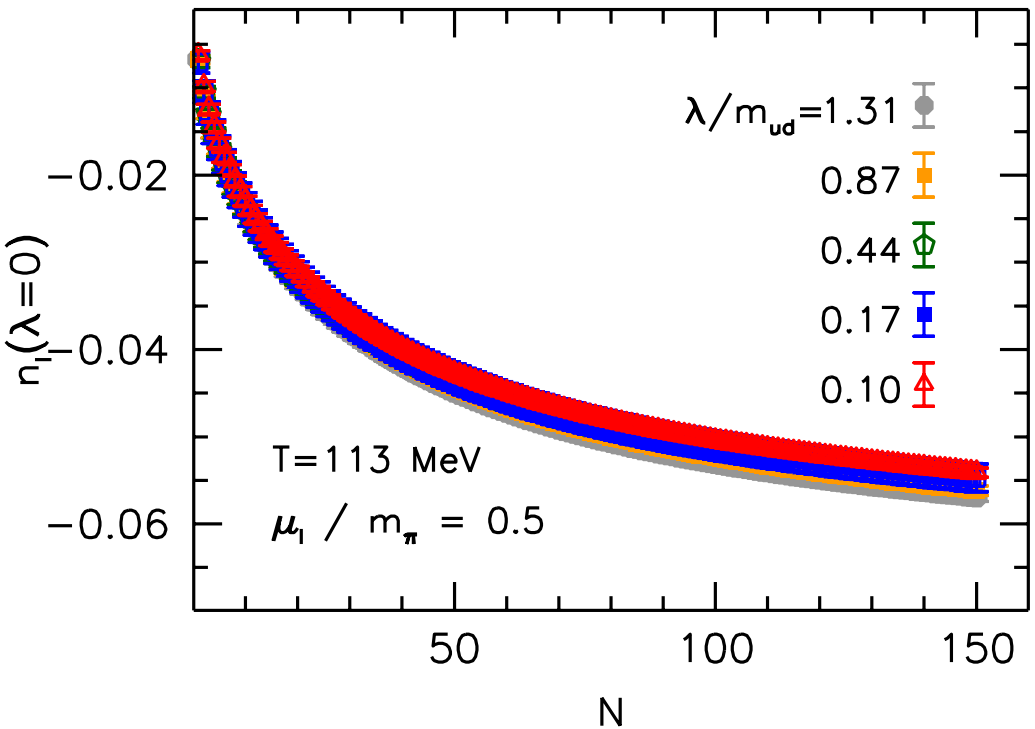
- spectral representation

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

Singular value representation

- spectral representation at $\lambda = 0$

$$n_I = \frac{2T}{V} \sum_{i=1}^{N} \mathrm{Re}\, \frac{\langle \psi_i | (\not{D}_\mu + m)^\dagger \not{D}'_\mu | \psi_i \rangle}{\xi_i^2}$$



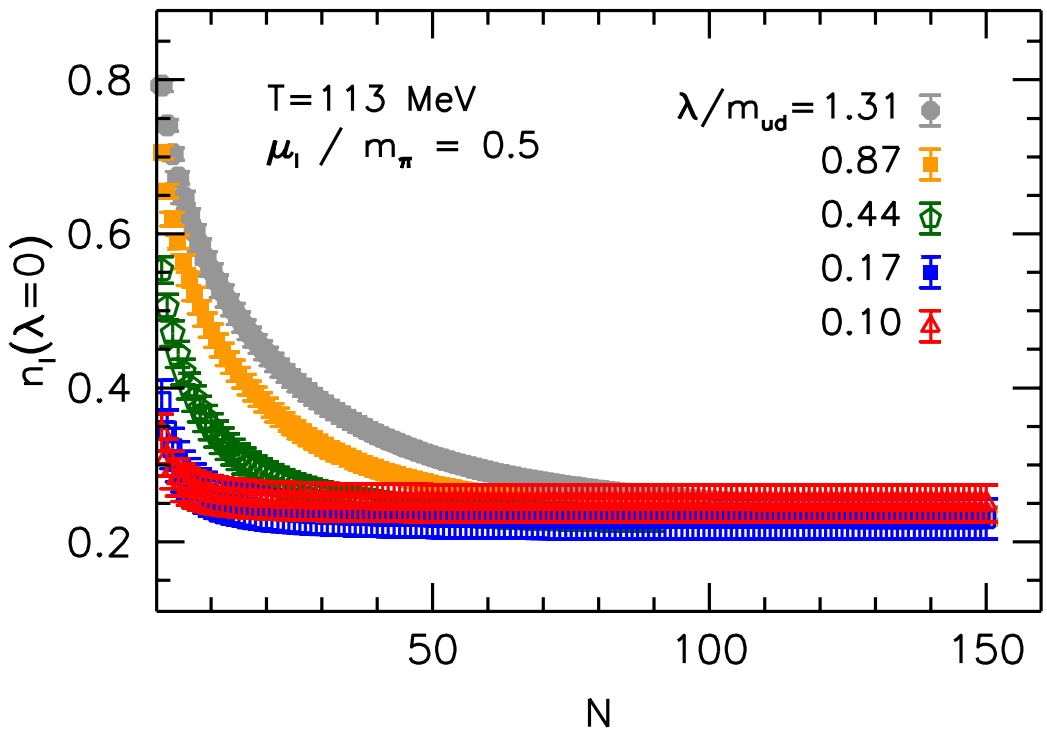
- convergence not visible for $N \leq 150$

Improvement

- work instead with the *difference*

$$\delta_{n_l} \equiv n_l(\lambda=0) - n_l(\lambda) = \frac{2T}{V} \sum_{i=1}^{N} \mathrm{Re}\langle\psi_i|(\not{D}_\mu + m)^\dagger \not{D}'_\mu|\psi_i\rangle \left[\frac{1}{\xi_i^2} - \frac{1}{\xi_i^2+\lambda^2}\right]$$

$$n_l(0) = n_l(\lambda) + \delta_{n_l}$$



- convergence already for small N

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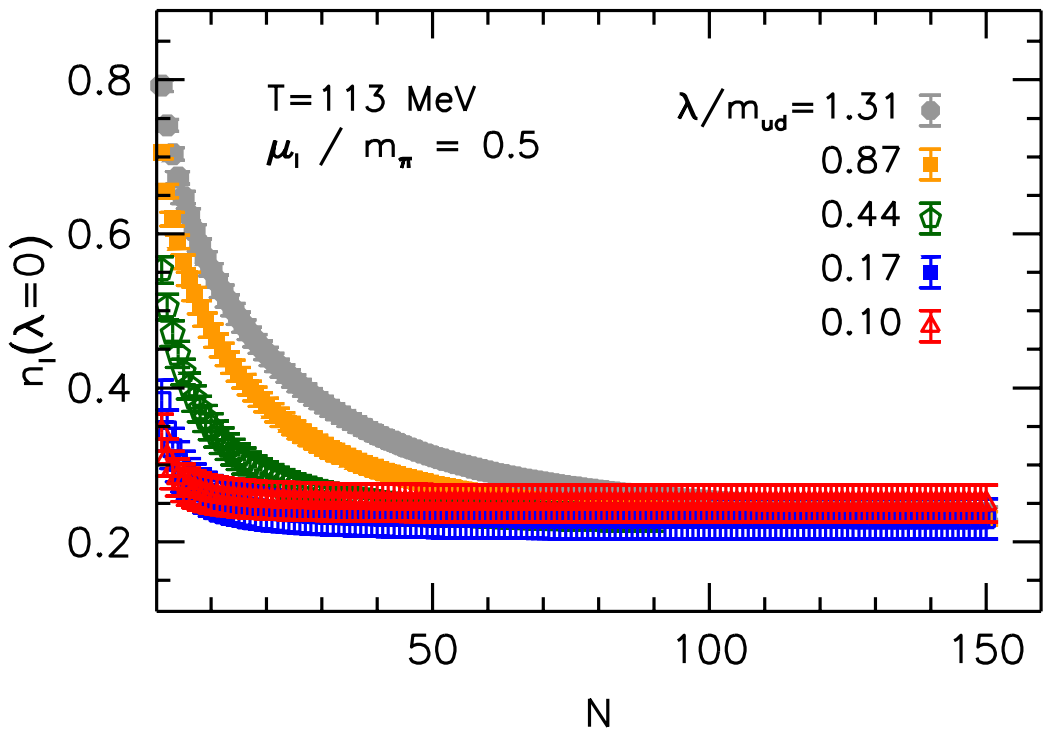
noisy estimators



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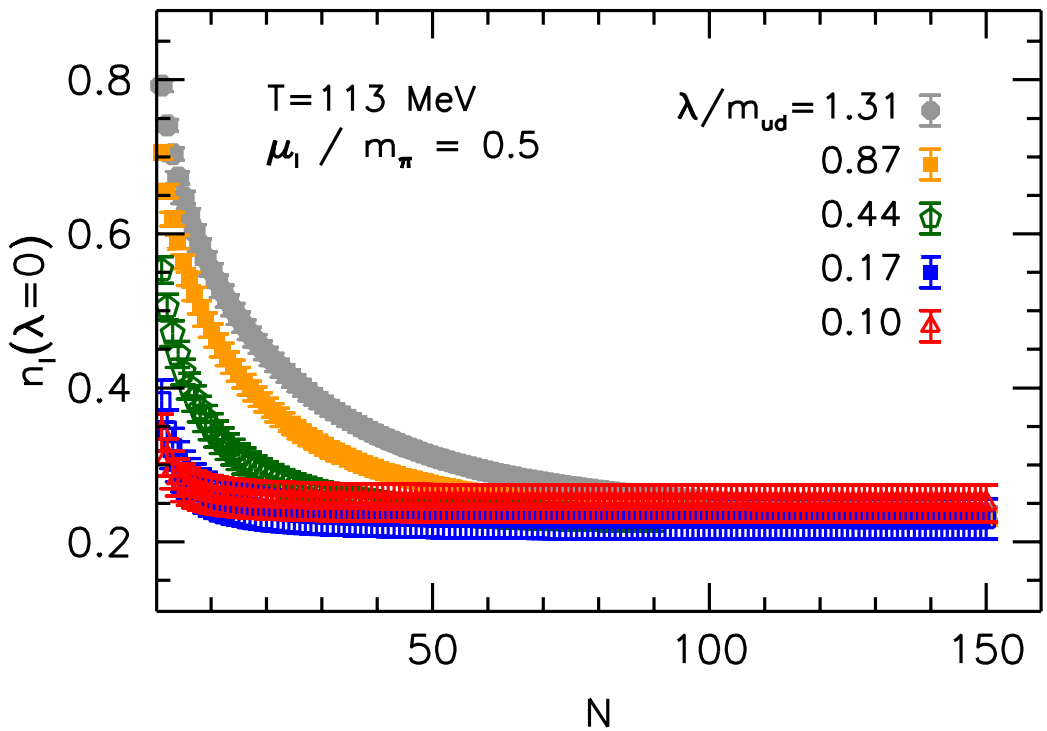


- convergence already for small N

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:

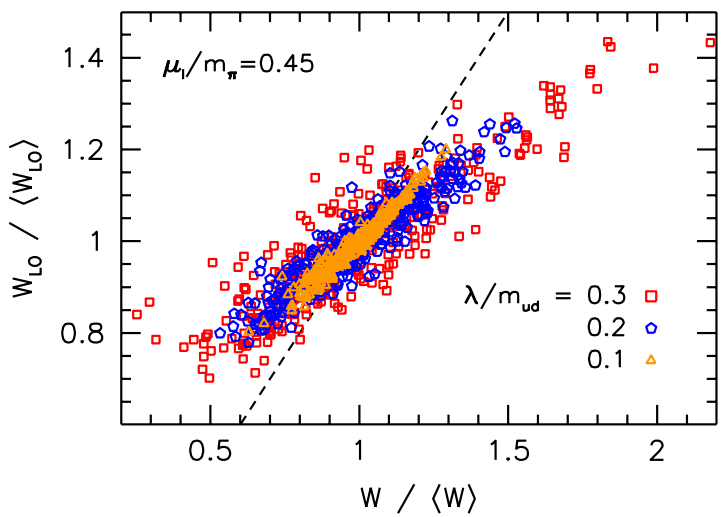
$$W_{\mathrm{LO}} = e^{-\lambda V_4 \pi}$$

- so we obtain

$$\langle \mathcal{O} \rangle_{\lambda=0} = \frac{\langle \mathcal{O} W_{\mathrm{LO}} \rangle_\lambda}{\langle W_{\mathrm{LO}} \rangle_\lambda} + \text{ higher orders in } \lambda$$

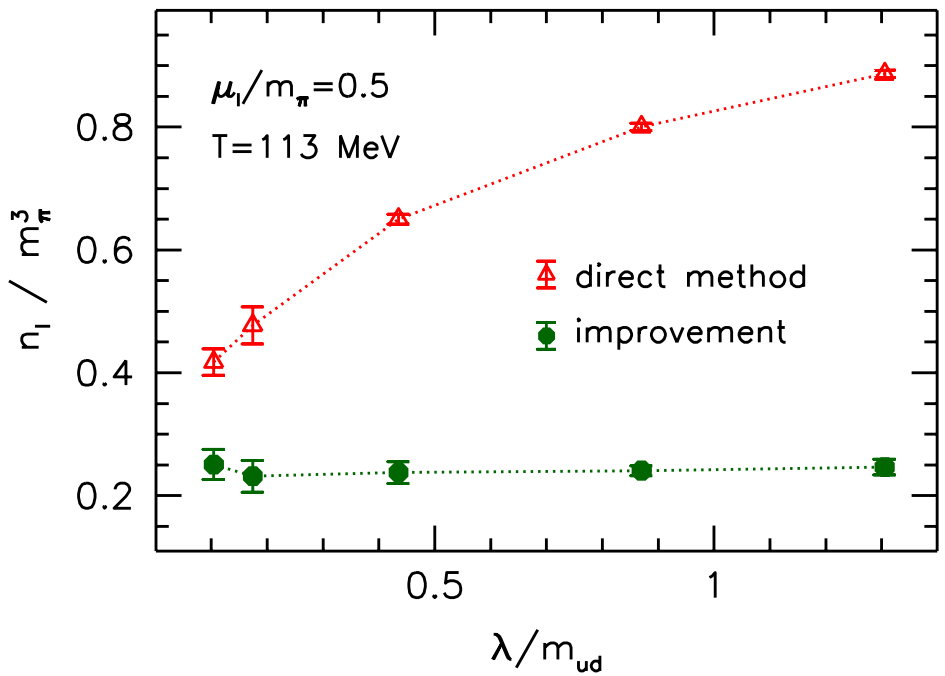
- W vs. W_{LO} scatter plot
- on small 8^4 lattices

  [Brandt, Endrődi, Schmalzbauer '18]



Impact of the improvement

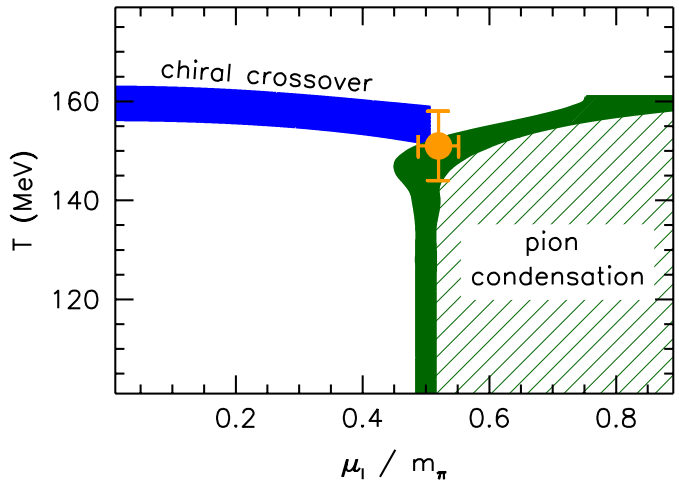
- improvement is crucial for reliable $\lambda \to 0$ extrapolation



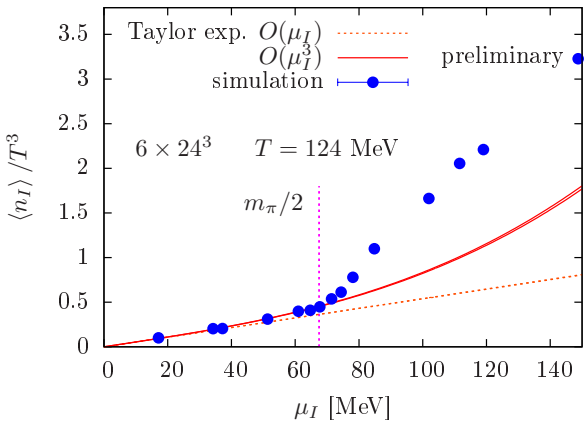
Results: Taylor vs. full

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



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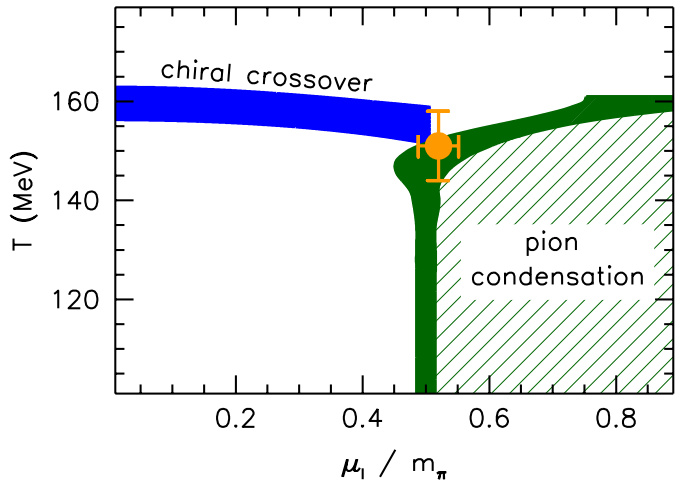

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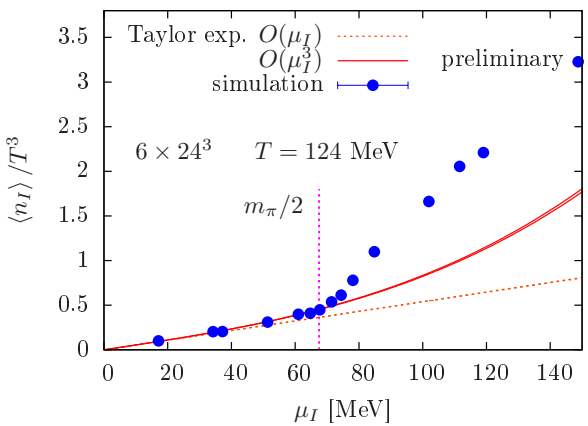

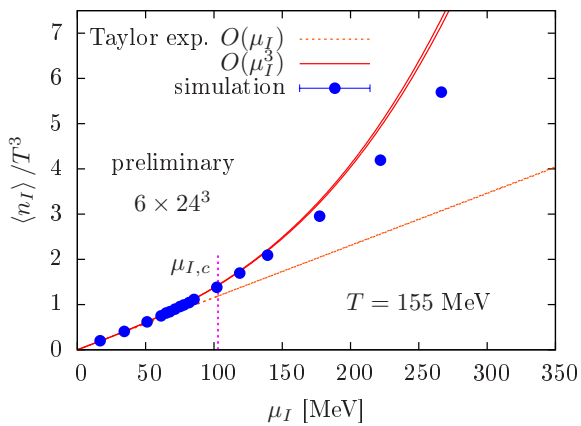

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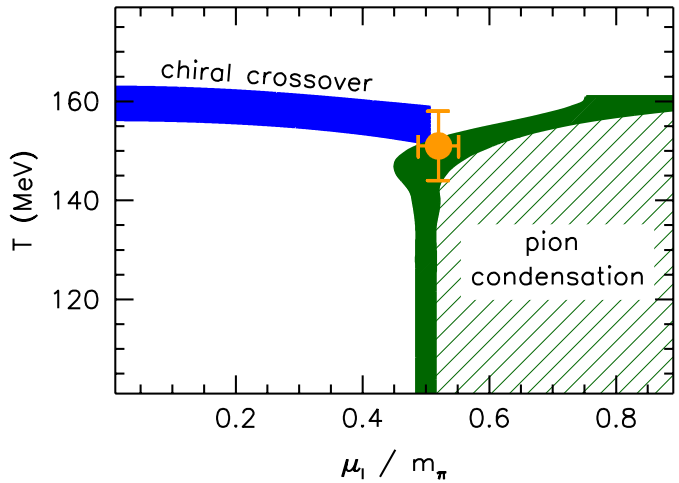

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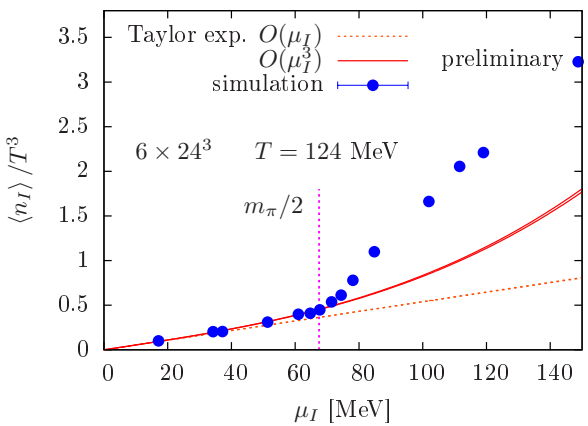
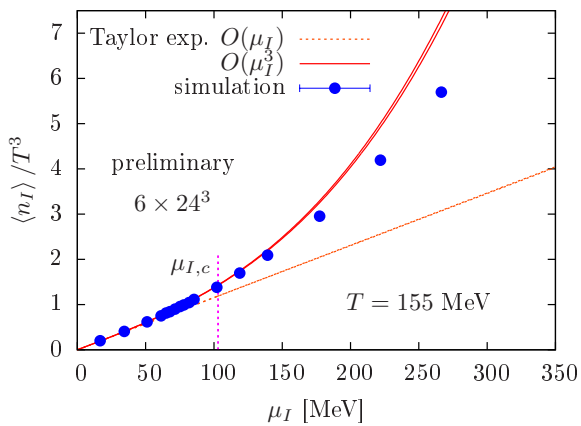
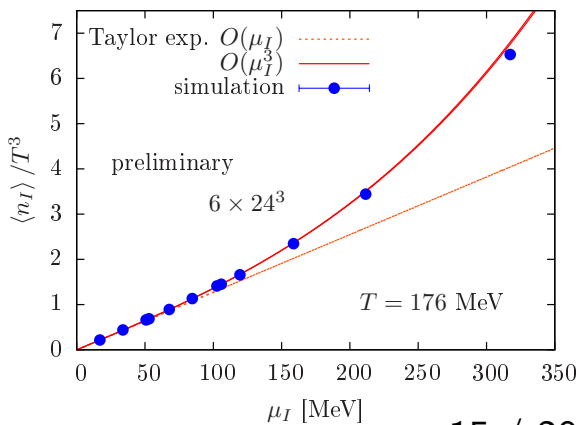






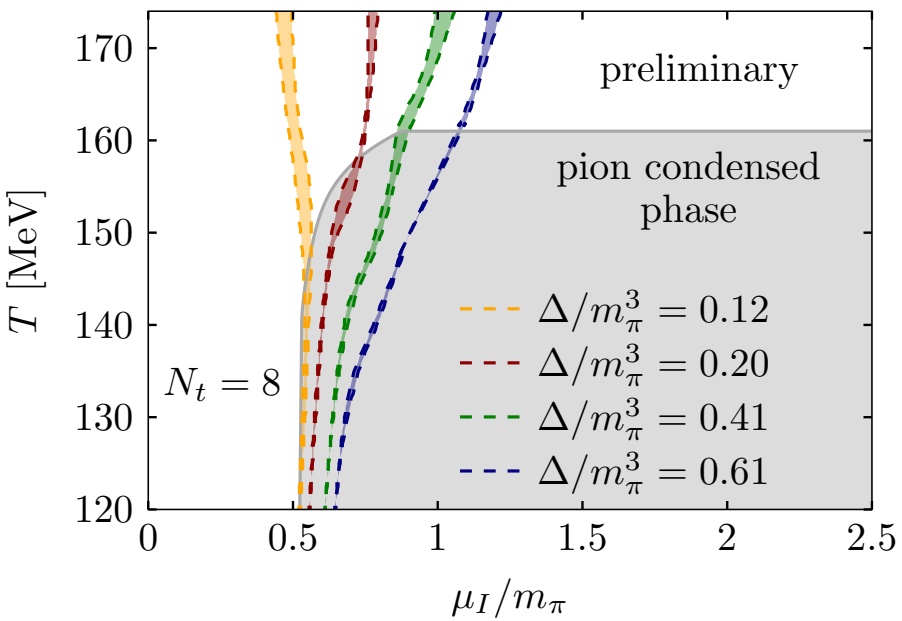
Reliability range

- quantify deviation between expanded and true values

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

- different behavior inside and outside pion condensed phase

leading order



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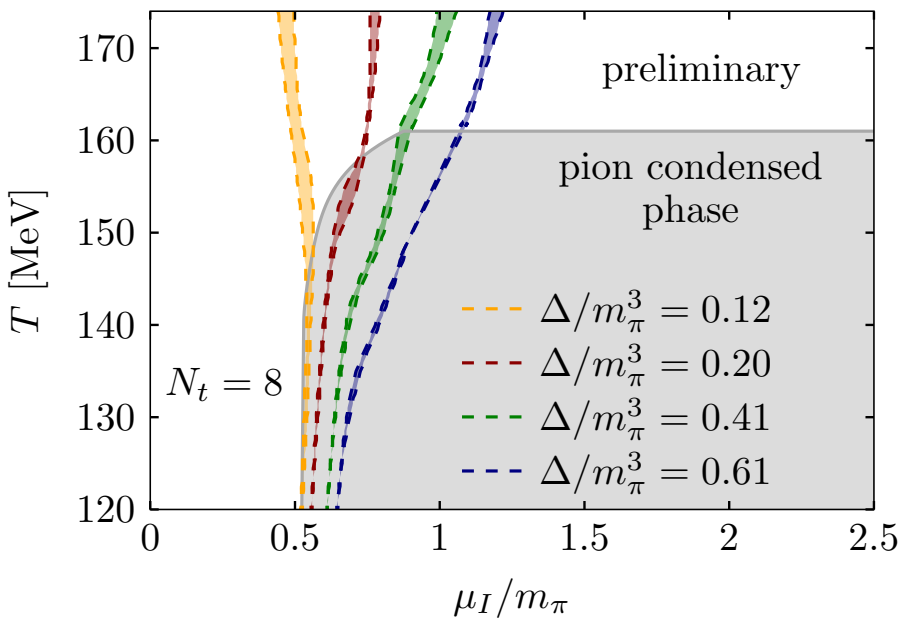
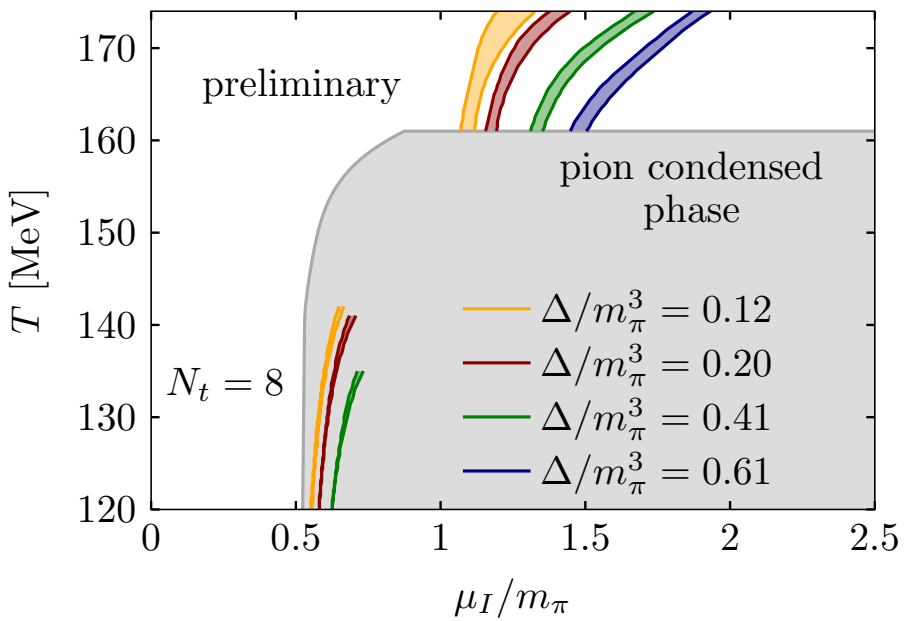
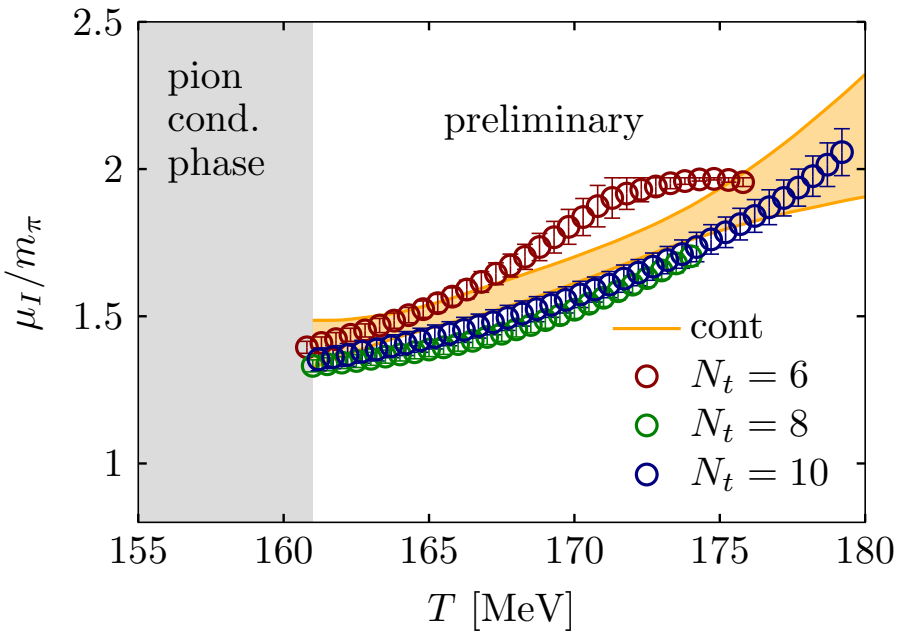


next-to-leading order

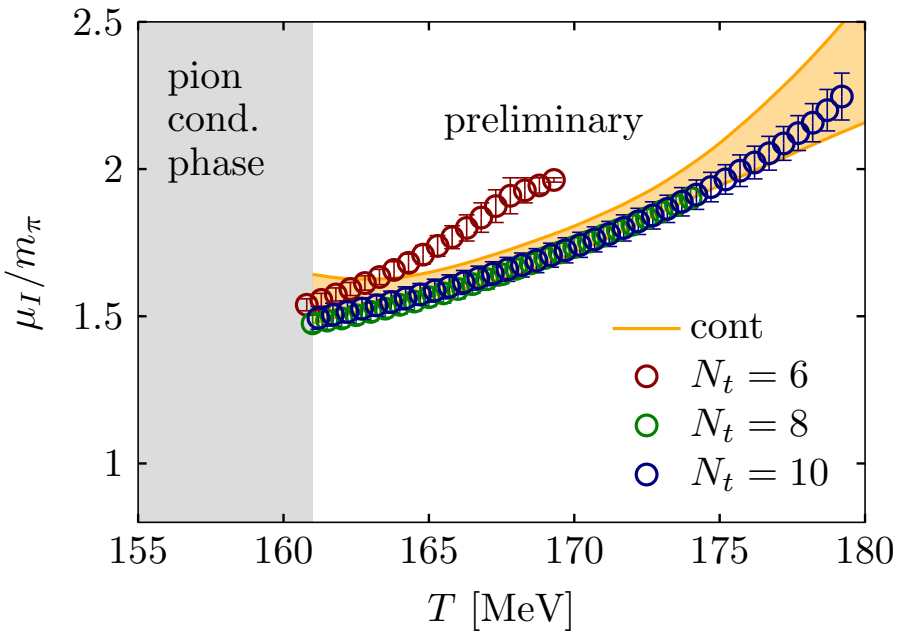


Towards the continuum

- preliminary continuum extrapolation shows similar trends for all lattice spacings



NLO, $\Delta = 0.41 m_\pi^3$



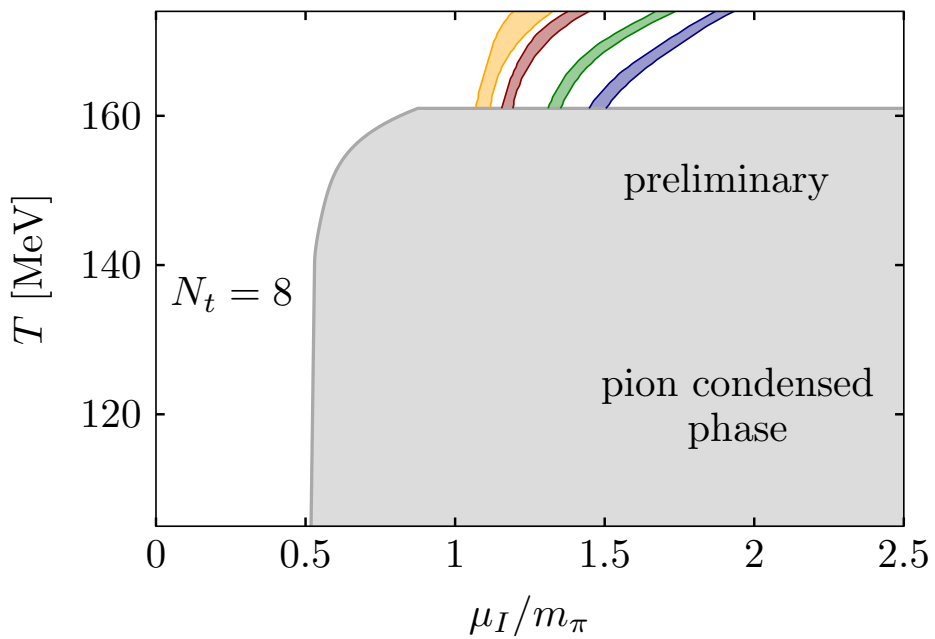
NLO, $\Delta = 0.61 m_\pi^3$

Radius of convergence

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

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

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



Radius of convergence

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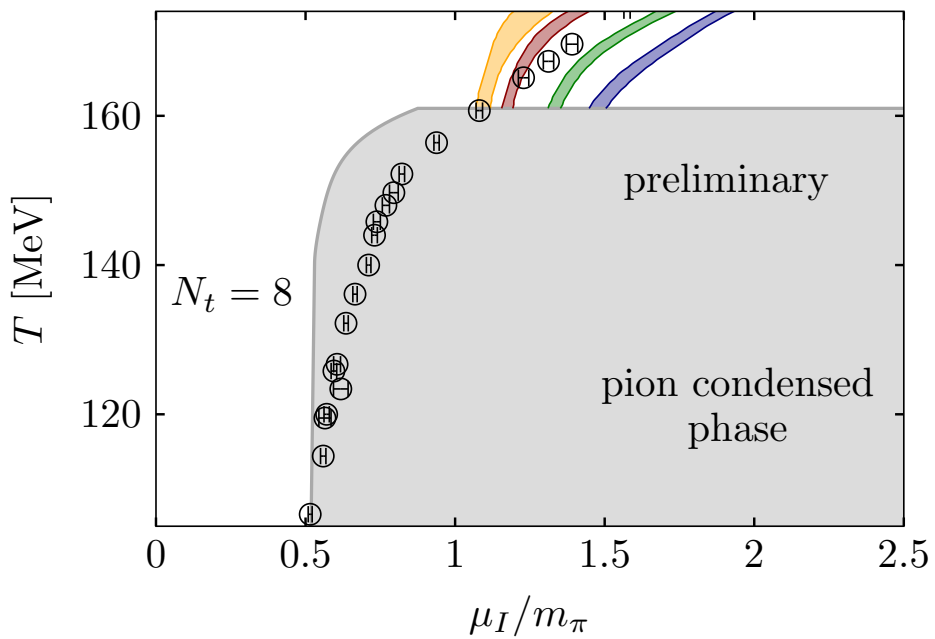
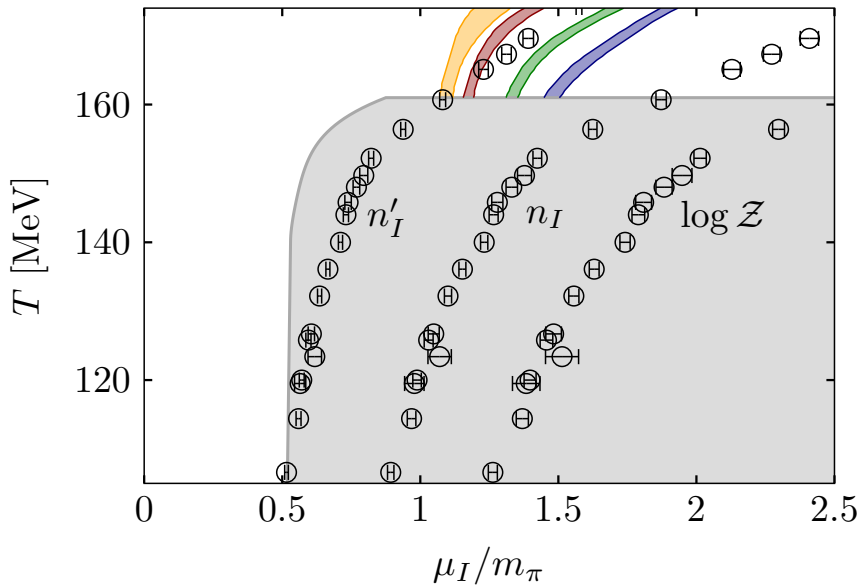


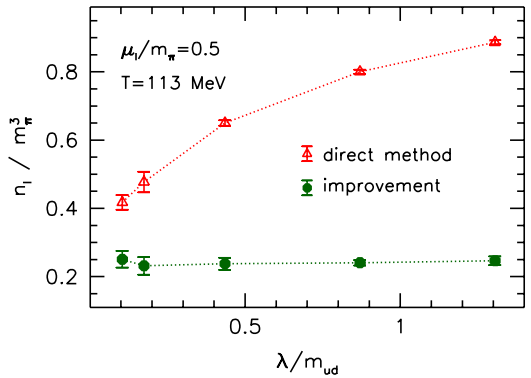
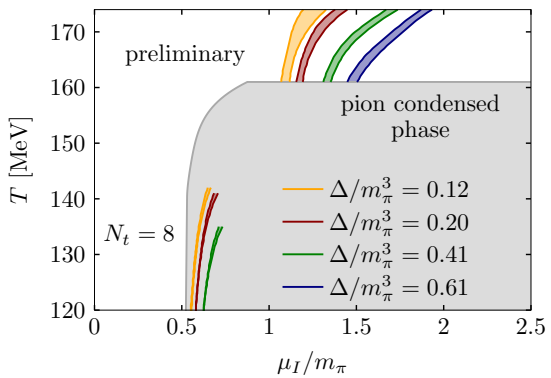
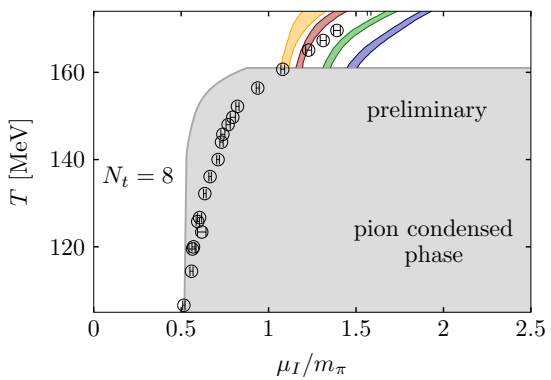
Remarks



- $r\{n'_I\} = r\{n_I\} = r\{\log \mathcal{Z}\}$, but leading estimators differ as
  $$1 \quad : \quad \sqrt{3} \quad : \quad \sqrt{6}$$
  susceptibility-series seems to converge faster
  (see also [Karsch, Schaefer, Wagner, Wambach '11])
- need higher-order estimates
- results may give insight to convergence properties at $\mu_B > 0$

Summary

- improve density using the singular values of $\not{D}_\mu + m$
  $\rightsquigarrow$ flat λ-extrapolation

- direct comparison to Taylor-expansions
  $\rightsquigarrow$ breakdown at phase transition
  $\rightsquigarrow$ reliability range for high T

- convergence radius estimator for isospin susceptibility close to phase boundary