Lattice QCD thermodynamics

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August 31 - September 03, 2021

Outline overall

- lecture 1: introduction to QCD and thermodynamics
- lecture 2: hot Yang-Mills theory on the lattice
- lecture 3: hot QCD on the lattice
- lecture 4: QCD in extreme conditions on the lattice

Outline lecture 4

- "rest" from lecture 3: Columbia-plot and full QCD EoS
- nonzero density in QCD and on the lattice
- sign problem and workarounds
- imaginary chemical potential

Center symmetry in full QCD

- perturbative effective potential again Roberge, Weiss NPB '86
- in Polyakov gauge

$$P = \mathrm{tr}\,\mathrm{diag}(e^{i\varphi_1}, e^{i\varphi_2}, e^{-i(\varphi_1+\varphi_2)})$$

  it is as if we had boundary conditions φ_i for the fermions
- in pure gauge theory we had three degenerate minima at

$$\varphi_1 = \varphi_2 = 0 \qquad \varphi_1 = \varphi_2 = 2\pi/3 \qquad \varphi_1 = \varphi_2 = -2\pi/3$$

- for fermions this shifts the Matsubara frequencies

$$\frac{\bar{\omega}_n}{T} \to (2n+1+0)\pi \qquad (2n+1+2/3)\pi \qquad (2n+1-2/3)\pi$$

  magnitude of lowest frequency is largest (so det M is largest) for

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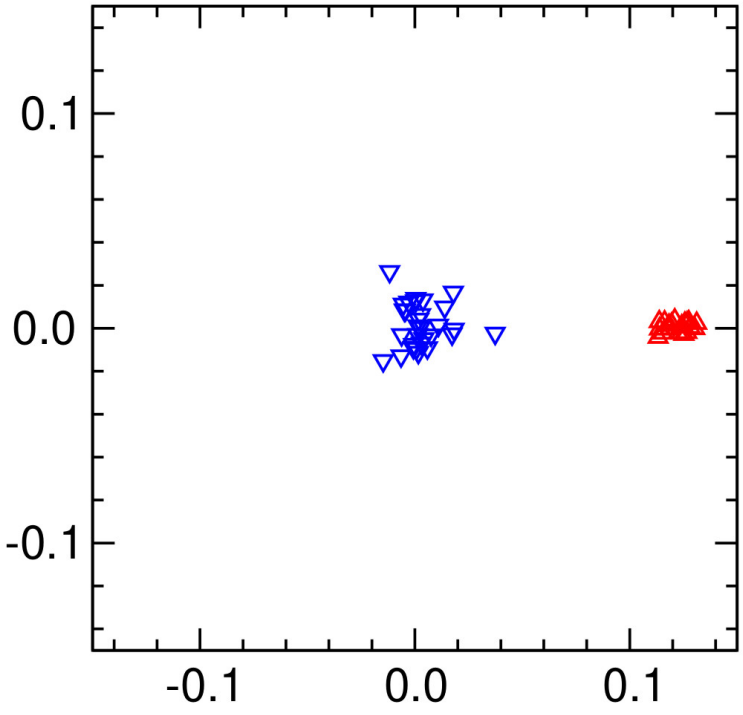
Polyakov loop in full QCD

- fermions prefer real Polyakov loops
  scatter plot at low T and high T

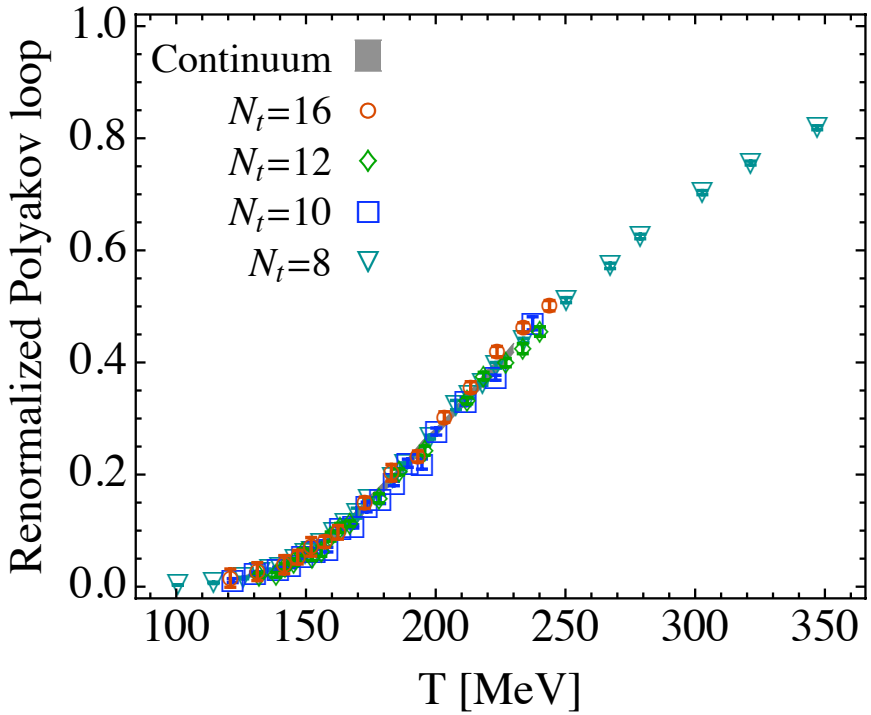


Dictionary 3.

	Ising model	QCD	
symm. group	$\mathrm{Z}(2)$	$\mathrm{Z}(3)$	$\mathrm{SU}(2)$
sp. breaking	$\langle M \rangle = \frac{\partial \log \mathcal{Z}}{\partial h}$	$\langle P \rangle$	$\langle \bar{\psi}_u \psi_u \rangle = \frac{\partial \log \mathcal{Z}}{\partial m_u}$
Goldstones	–	–	3
exp. breaking	$h > 0$	$m_u = m_d < \infty$	$m_u = m_d > 0$
symm. restoration	at high T	at low T	at high T

Results: Polyakov loop in full QCD

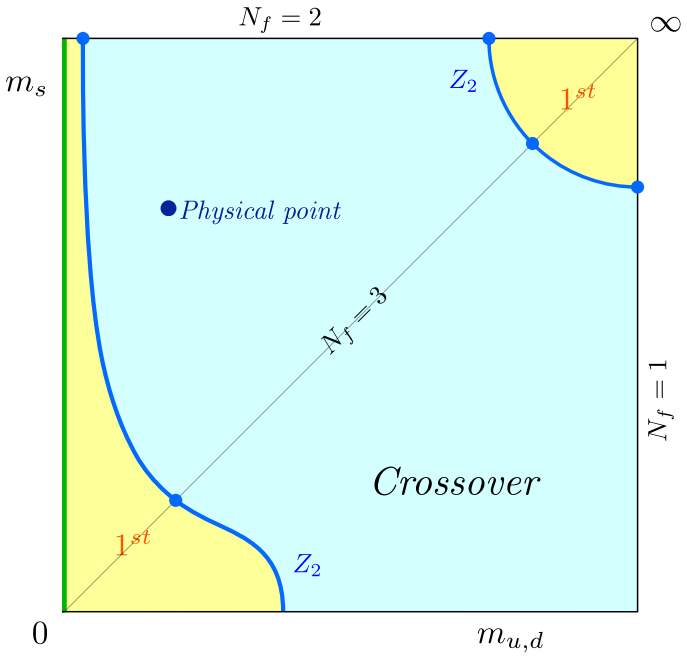
- fixed N_t-approach Borsányi et al. JHEP '10



- chiral symmetry restoration at $\approx (155 \pm 15)$ MeV
- deconfinement in roughly same region

Columbia-plot

- full QCD at the physical point has no exact symmetries
  not quite $\mathrm{SU}(2)$ chirally symmetric because $m_u, m_d > 0$
  not quite $\mathrm{Z}(3)$ center symmetric because $m_f < \infty$
- order of finite temperature transition as a function of $m_u = m_d$ and m_s: Columbia-plot Brown et al. PLB '90



Cuteri et al. PRD '18

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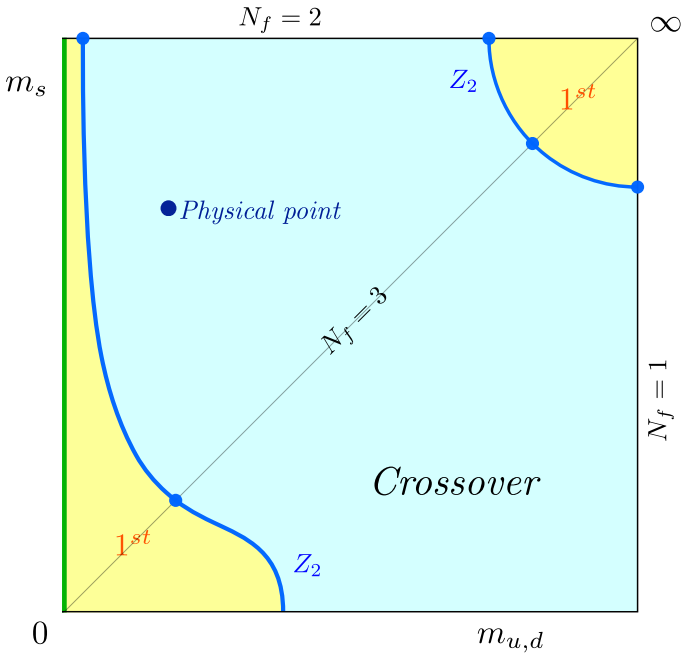
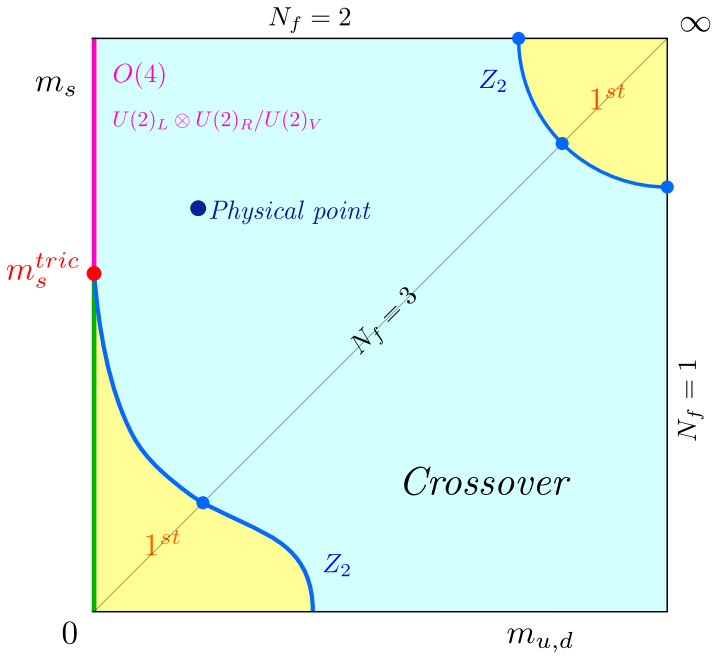




Cuteri et al. PRD '18

Equation of state

Integral method in QCD

- remember in pure gauge theory

$$\log \mathcal{Z}(\beta_1) - \log \mathcal{Z}(\beta_0) = \int_{\beta_0}^{\beta_1} \mathrm{d}\beta \, \frac{\partial \log \mathcal{Z}}{\partial \beta}$$

- now more parameters: β, m_f but they are not independent

$$\boxed{a(\beta)} \qquad \boxed{m_f(\beta)}$$

- therefore

$$\log \mathcal{Z}(\beta_1, m_f(\beta_1)) - \log \mathcal{Z}(\beta_0, m_f(\beta_0)) = \int_{\beta_0}^{\beta_1} \mathrm{d}\beta \left[\frac{\partial \log \mathcal{Z}}{\partial \beta} + \sum_f \frac{\partial \log \mathcal{Z}}{\partial m_f} \frac{\partial m_f}{\partial \beta} \right]$$

gauge action $\langle S_G \rangle$ as well as condensates $\langle \bar{\psi}_f \psi_f \rangle$ enter

Integral method in QCD

- renormalization same as for pure gauge theory

$$\frac{p^{\mathrm{r}}(T_1)}{T_1^4} - \frac{p^{\mathrm{r}}(T_0)}{T_0^4} = \frac{N_t^3}{N_s^3}\int_{\beta_0}^{\beta_1} \mathrm{d}\beta \Big[-\langle S_G\rangle_{N_s^3 N_t} + \langle S_G\rangle_{N_s^4} + \sum_f \left(\langle\bar\psi_f\psi_f\rangle_{N_s^3 N_t} - \langle\bar\psi_f\psi_f\rangle_{N_s^4}\right)\frac{\partial m_f}{\partial\beta}\Big]$$

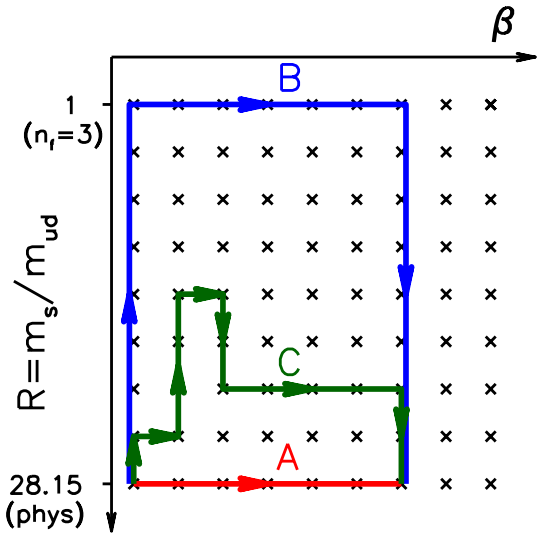
with starting point β_0 where $p^{\mathrm{r}}(T_0)/T_0^4 \approx 0$

- renormalized interaction measure

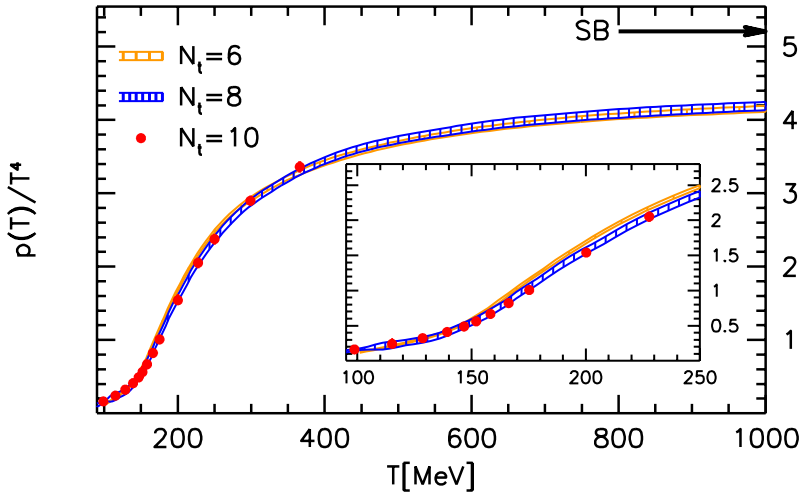
$$\frac{I^{\mathrm{r}}}{T^4} = \frac{N_t^3}{N_s^3}\frac{a(\beta)}{a'(\beta)}\left[\langle S_G\rangle_{N_s^3 N_t} - \langle S_G\rangle_{N_s^4} + \sum_f \left(\langle\bar\psi_f\psi_f\rangle_{N_s^3 N_t} - \langle\bar\psi_f\psi_f\rangle_{N_s^4}\right)\frac{\partial m_f}{\partial\beta}\right]$$

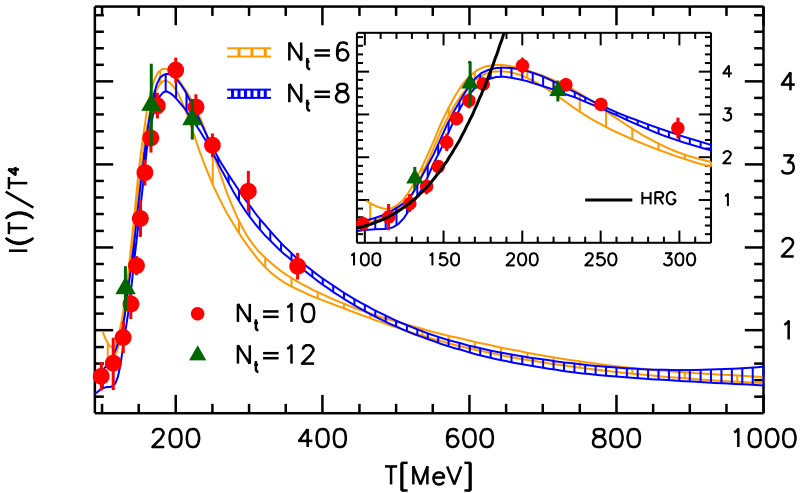
Integration paths

- integral is independent of integration path



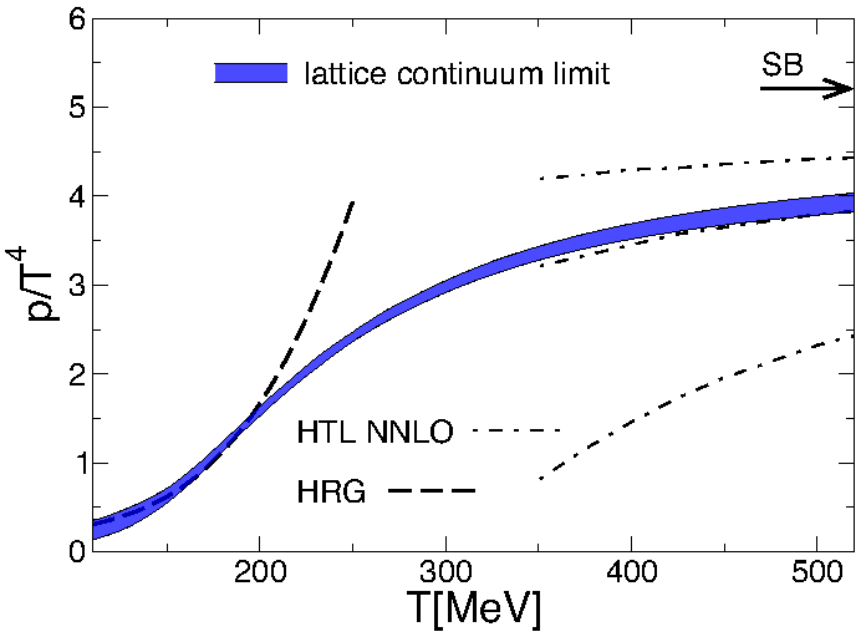
- averaging over different paths Borsányi, Endrődi et al. JHEP '10

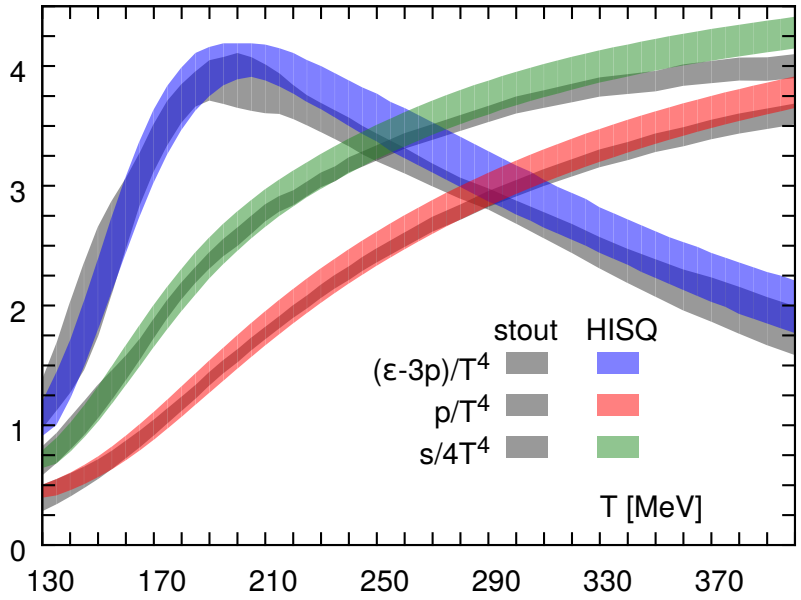




Results: equation of state

- most recent results using two different staggered discretizations Borsányi et al. PLB '14 Bazavov et al. PRD '14





- low T: agreement with Hadron Resonance Gas model
  high T: comparison to Hard Thermal Loop resummed perturbation theory

QCD at nonzero density

Chemical potential in the continuum

- Noether current for $\mathrm{U}_V(1)$ symmetry

$$\psi \to e^{i\alpha}\psi \qquad \partial_\nu \bar{\psi}\gamma_\nu\psi = 0 \qquad \hat{N} = \int \mathrm{d}^3\mathbf{x}\, \bar{\psi}\gamma_4\psi \qquad \frac{\mathrm{d}\hat{N}}{\mathrm{d}t} = [\hat{H}, \hat{N}] = 0$$

- canonical path integral

$$Z_N = \mathrm{tr}\left[e^{-\hat{H}/T}\delta_{\hat{N},N}\right]$$

- grand canonical path integral

$$\mathcal{Z}(\mu) = \mathrm{tr}\, e^{-(\hat{H}-\mu\hat{N})/T} = \int \mathcal{D}A_\nu\, \mathcal{D}\bar{\psi}\, \mathcal{D}\psi\, e^{-S_G - S_F(\mu)}$$

with

$$S_F(\mu) = S_F(0) + \mu \int \mathrm{d}^4x\, \bar{\psi}\gamma_4\psi \qquad \to \qquad \not{D}(\mu) = \not{D}(0) + \mu\gamma_4$$

Grand canonical equation of state

- free energy (density)

$$F(T,\mu) = -T \log \mathcal{Z} \qquad f = \frac{F}{V}$$

- entropy density

$$s = -\frac{1}{V}\frac{\partial F}{\partial T}$$

- pressure

$$p = -\frac{\partial F}{\partial V} \xrightarrow{V\to\infty} -f$$

- number density

$$n = -\frac{1}{V}\frac{\partial F}{\partial \mu}$$

- energy density

$$\epsilon - \mu n = -\frac{1}{V}\frac{\partial \log \mathcal{Z}}{\partial (1/T)} = f + Ts$$

- interaction measure / trace anomaly

$$I = \mathrm{tr}\, T_{\mu\nu} = \epsilon - 3p$$

Chemical potential in the free case

- in the Dirac operator $\partial_4 \to \partial_4 + \mu$
- Matsubara frequencies are shifted $\bar{\omega}_n \to \bar{\omega}_n - i\mu$
- same tricks as used at $\mu = 0$ lead to

$$f = -2 \int \frac{\mathrm{d}^3\mathbf{p}}{(2\pi)^3} \left[E_p + T \log(1 + e^{-(E_p+\mu)/T}) + T \log(1 + e^{-(E_p-\mu)/T}) \right]$$

- finite combinations:

$$f(T,\mu) - f(0,0) \qquad \text{or} \qquad f(T,\mu) - f(T,0)$$

- note: imaginary chemical potentials $\mu = i\theta$ have periodicity

$$f(\theta) = f(\theta + 2\pi T)$$

also clear from Matsubara frequencies: $(2n+1)\pi T + \theta$

Chemical potential on the lattice

Chemical potential on the lattice

- add $\mu\gamma_4$ to Dirac operator

$$\not{D} = \frac{1}{2}\sum_{\nu}\gamma_\nu \left[\underset{\nu}{\longrightarrow} - \underset{\nu}{\longleftarrow} \right] + \mu\gamma_4 \bullet$$

- in the free case ($U_\mu = \mathbb{1}$) $\log\det M$ contains divergences

  Hasenfratz, Karsch PLB '83

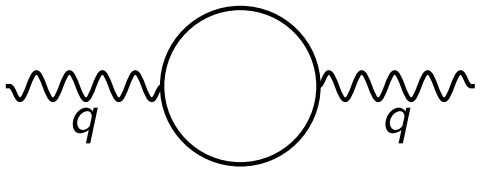
$$\log\det M_{\text{free}}(\mu) = \mathcal{O}(a^{-4}) + \mathcal{O}(m^2 a^{-2}) + \mathcal{O}(m^4 \log a) + \mathcal{O}(\mu^2 a^{-2})$$

  so the number density

$$n = \mathcal{O}(\mu a^{-2})$$

- but in the continuum the number density is finite (0 at $T = 0$)

$$n \propto \Pi_{00}(q = 0) =$$



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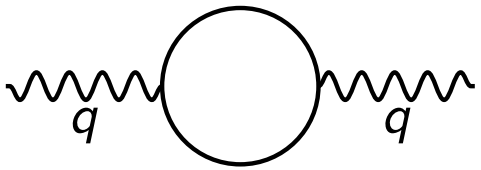

  did we violate gauge invariance?

Chemical potential on the lattice

- imaginary chemical pot. as 4th component of $\mathrm{U}(1)$ gauge field

$$\not{D} + i\theta\gamma_4 = \not{D} + i\not{\mathcal{A}} \qquad \mathcal{A}_\nu = \theta\delta_{\nu 4}$$

- just like gluon field, via parallel transporters

  Hasenfratz, Karsch PLB '83

$$u_\mu = \exp(i\mathcal{A}_\mu) \in \mathbb{U}(1)$$

- multiplying the $\mathrm{SU}(3)$ links (imaginary μ)

$$\not{D} = \frac{1}{2}\sum_i \gamma_i \left[\xrightarrow[i]{} - \xleftarrow[i]{} \right] + \frac{1}{2}\gamma_4 \left[\xrightarrow[t]{e^{i\theta}} - \xleftarrow[t]{e^{-i\theta}} \right]$$

- no μ-dependent divergences in $\log\det M_{\mathrm{free}}$ ✓

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- multiplying the $\mathrm{SU}(3)$ links (real μ)

$$\not{D} = \frac{1}{2}\sum_i \gamma_i \left[\xrightarrow[i]{} - \xleftarrow[i]{} \right] + \frac{1}{2}\gamma_4 \left[\xrightarrow[t]{e^{\mu}} - \xleftarrow[t]{e^{-\mu}} \right]$$

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Sign problem

Chemical potential and unitarity

- staggered quarks again
- imaginary chemical potential

$$\not{D}_{nm} = \frac{1}{2a} \sum_{\nu} \eta_\nu(n) \left[U_\nu(n) e^{i\theta\delta_{\nu 4}} \delta_{n+\hat{\nu},m} - U_\nu^\dagger(n-\hat{\nu}) e^{-i\theta\delta_{\nu 4}} \delta_{n-\hat{\nu},m} \right]$$

  links still unitary

- real chemical potential

$$\not{D}_{nm} = \frac{1}{2a} \sum_{\nu} \eta_\nu(n) \left[U_\nu(n) e^{\mu\delta_{\nu 4}} \delta_{n+\hat{\nu},m} - U_\nu^\dagger(n-\hat{\nu}) e^{-\mu\delta_{\nu 4}} \delta_{n-\hat{\nu},m} \right]$$

  forward/backward propagation enhanced/suppressed
  links <u>not</u> unitary anymore

Sign problem

- now {forward hopping} $\neq$ {backward hopping}†

$$\eta_5 \not{D}(\mu)\eta_5 = \not{D}^\dagger(-\mu)$$

  η_5-hermiticity is lost $\Rightarrow$ det $M(\mu) \in \mathbb{C}$
- path integral

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

  no probabilistic interpretation anymore
- complex action problem
- actually we know $\mathcal{Z} \in \mathbb{R}$

$$\mathcal{Z} = \int \mathcal{D}U\ \mathrm{Re}[\det M(\mu)]^{1/4}\, e^{-\beta S_G}$$

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- sign problem
- bonus staggered problem: ambiguous complex rooting

Sign problem - workarounds

- here: brief description of
  - reweighting
  - analytical continuation from $i\mu = \theta$
- many other approaches
  - Taylor expansion in μ around $\mu = 0$
  - complex Langevin
  - Lefschetz thimbles

Reweighting

- determinant is complex

$$\det M = |\det M|\, e^{i\phi}$$

- replace complex weight by real weight

$$\langle A \rangle = \frac{\int \mathcal{D}U \, \det M \, e^{-\beta S_G} A[U]}{\int \mathcal{D}U \, \det M \, e^{-\beta S_G}} = \frac{\int \mathcal{D}U \, |\det M| \, e^{-\beta S_G} A[U] \, e^{i\phi}}{\int \mathcal{D}U \, |\det M| \, e^{-\beta S_G} \, e^{i\phi}}$$
$$= \frac{\int \mathcal{D}U \, |\det M| \, e^{-\beta S_G} A[U] \, e^{i\phi}}{\int \mathcal{D}U \, |\det M| \, e^{-\beta S_G}} \Bigg/ \frac{\int \mathcal{D}U \, |\det M| \, e^{-\beta S_G} \, e^{i\phi}}{\int \mathcal{D}U \, |\det M| \, e^{-\beta S_G}}$$

- these are *phase quenched* expectation values

$$\langle A \rangle = \frac{\langle A \, e^{i\phi} \rangle_{\mathrm{pq}}}{\langle e^{i\phi} \rangle_{\mathrm{pq}}}$$

- sign problem is solved. Or is it?

Overlap problem

- overlap problem

$$\langle e^{i\phi}\rangle_{\rm pq} = \frac{\mathcal{Z}}{\mathcal{Z}_{\rm pq}} = \exp\left[-\frac{V}{T}(f - f_{\rm pq})\right]$$

exponentially small in V

$$\langle A\rangle \sim \frac{0}{0} \qquad \text{for large volumes} \qquad ↯$$

- note

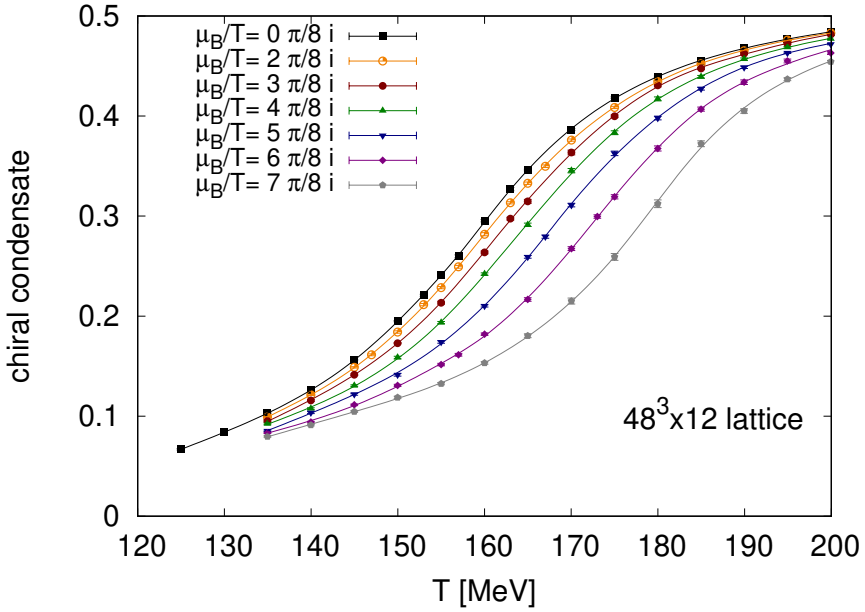
$$|\det M(\mu)| = \sqrt{\det M(\mu)\cdot[\det M(\mu)]^*} = \sqrt{\det M(\mu)\cdot\det M(-\mu)}$$

phase quenched ensemble corresponds to *isospin* chemical potential setting

$$\mu_d = -\mu_u$$

Analytic continuation

- perform simulations at $\mu^2 < 0$ Borsányi et al. PRL '20



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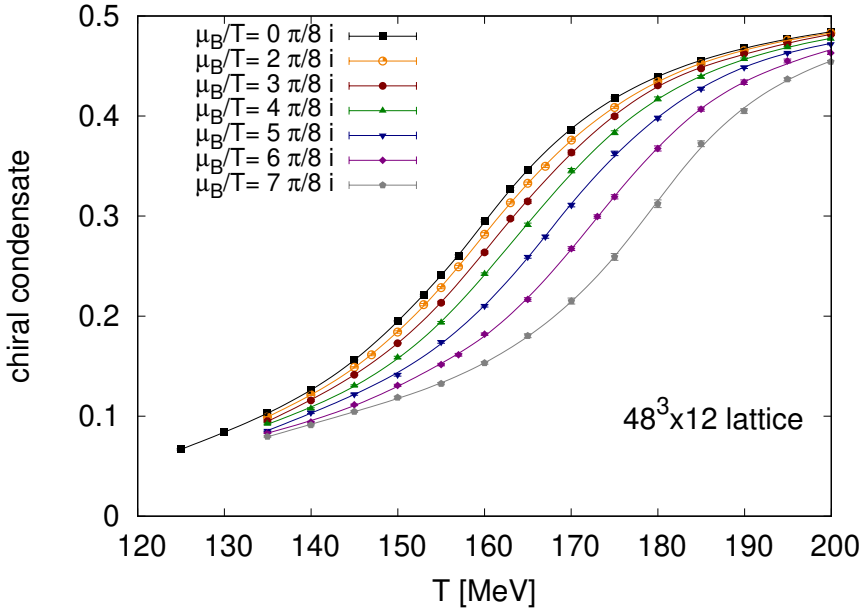
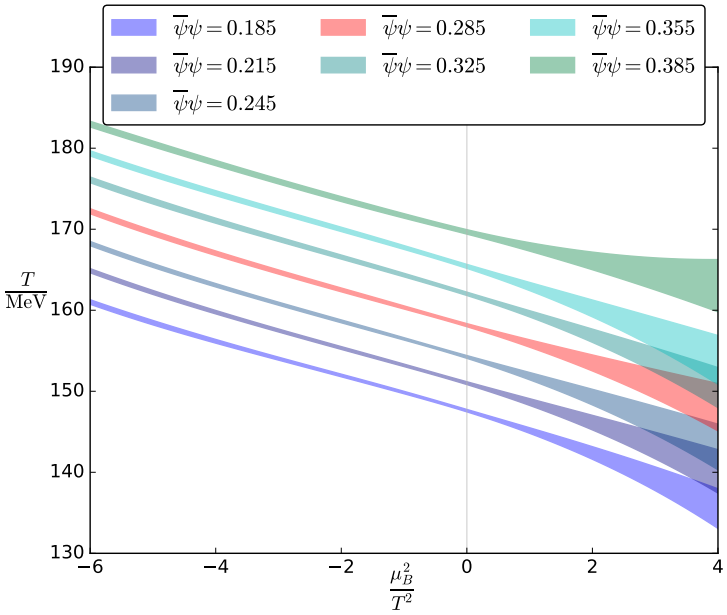


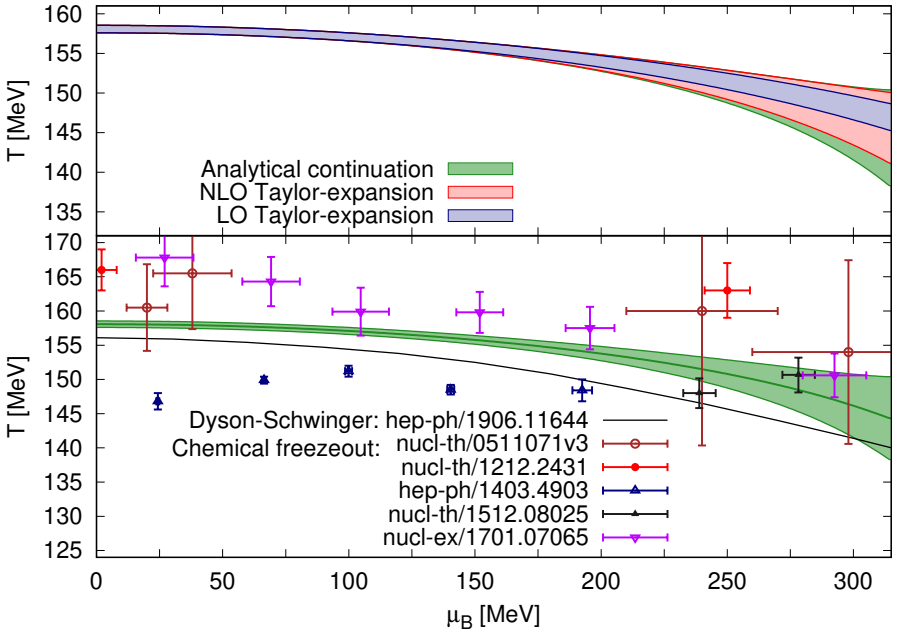


- fit and analytically continue to $\mu^2 > 0$

Phase diagram

- analytically continue susceptibility peak positions

  Borsányi et al. PRL '20



Roberge-Weiss transitions

Imaginary chemical potentials

- remember center sectors (Polyakov loop eigenvalues)

$$\varphi_1 = \varphi_2 = 0 \qquad \varphi_1 = \varphi_2 = 2\pi/3 \qquad \varphi_1 = \varphi_2 = -2\pi/3$$

shifting the Matsubara frequencies

$$\frac{\bar{\omega}_n + \theta}{T} \to (2n{+}1{+}\theta{+}0)\pi \qquad (2n{+}1{+}\theta{+}2/3)\pi \qquad (2n{+}1{+}\theta{-}2/3)\pi$$

- magnitude of lowest frequency is largest for:

Imaginary chemical potentials

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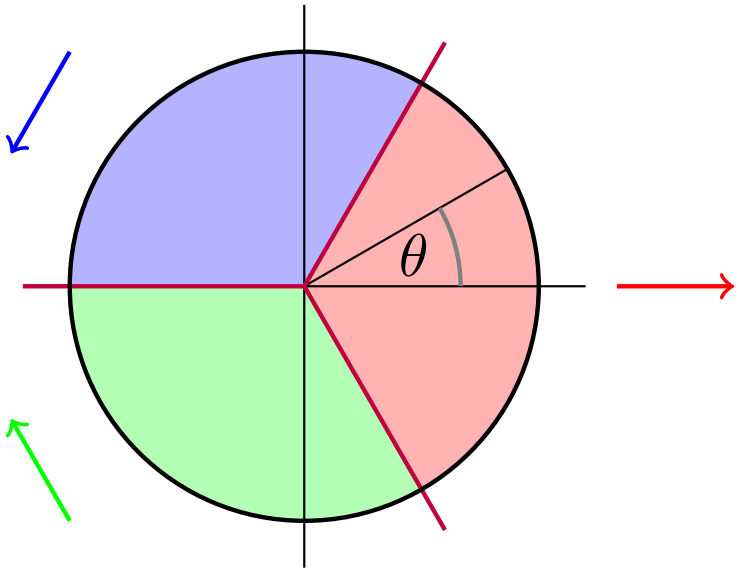
- magnitude of lowest frequency is largest for:

$-\pi T/3 < \theta < \pi T/3$	$\varphi = 0$
$\pi T/3 < \theta < \pi T$	$\varphi = -2\pi/3$
$-\pi T < \theta < -\pi T/3$	$\varphi = 2\pi/3$

Roberge-Weiss transitions

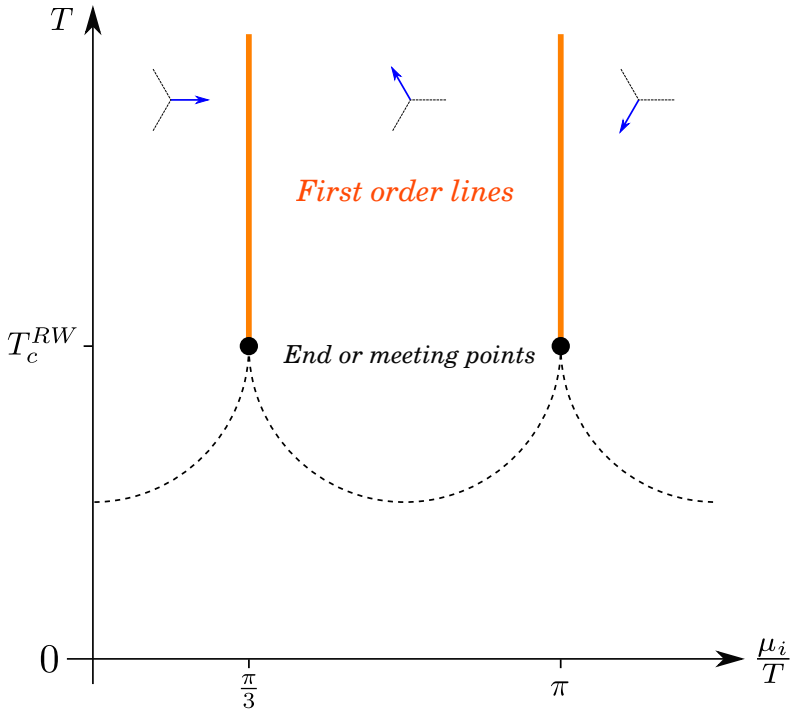
- preferred center sectors at nonzero θ



- $f(\theta + 2\pi T) = f(\theta)$ periodicity already in free case
- in QCD $f(\theta + 2\pi T/3) = f(\theta)$
  (only $N\%3 = 0$ states allowed) Roberge, Weiss NPB '86

Roberge-Weiss transitions

- phase diagram at nonzero θ



Roberge, Weiss NPB '86 Czaban et al. PRD '16

- analytical continuation limited by $\theta < \pi T/3$ at high temperature
- note: ongoing research on RW endpoint