Lattice QCD in extreme conditions

Gergely Endrődi

University of Bielefeld

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Outline overall

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

Outline lecture 3

- dynamical fermions and chiral symmetry; staggered fermions
- finite temperature transition in full QCD
- equation of state
- nonzero density and the sign problem

Dynamical fermions

Full QCD path integral

- path integral over links and fermion fields

$$\mathcal{Z} = \int \mathcal{D}U\, \mathcal{D}\bar{\psi}\, \mathcal{D}\psi\, e^{-\beta S_G - \bar{\psi} M \psi}$$

- Grassmann numbers on a computer?
  $\Rightarrow$ integrate out fermions analytically

$$\mathcal{Z} = \int \mathcal{D}U \,\det M\, e^{-\beta S_G}$$

- fermion matrix

$$M = \mathrm{diag}(\not{D} + m_u, \not{D} + m_d, \not{D} + m_s, \ldots)$$

- note: $m_f \to \infty$ of full QCD gives back pure gauge theory

Staggered fermions

- naive Dirac operator: 16-fold doubling

$$\not{D} = \frac{1}{2} \sum_{\mu} \gamma_\mu \left[\xrightarrow[\mu]{} - \xleftarrow[\mu]{} \right]$$

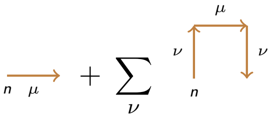
- staggered Dirac operator (no Dirac indices!): 4-fold doubling

$$\not{D} = \frac{1}{2} \sum_{\mu} \eta_\mu \left[\xrightarrow[\mu]{} - \xleftarrow[\mu]{} \right] \qquad \eta_\mu(n) = (-1)^{\sum_{\nu<\mu} n_\nu}$$

- partition function

$$\mathcal{Z} = \int \mathcal{D}U \, e^{-\beta S_G} \prod_f \sqrt[4]{\det(\not{D} + m_f)}$$

- rooting: no doubling? but has theoretical problems Creutz '07
- note: local averaging of links suppresses discretization errors
  "stout smearing" Morningstar, Peardon PRD '04



Staggered η_5-hermiticity

- γ_5-hermiticity $\quad \{\text{forward hopping}\} = \{\text{backward hopping}\}^\dagger$

$$\boxed{\gamma_5 \not{D} \gamma_5 = \not{D}^\dagger}$$

- determinant is real

$$\det[\gamma_5 \not{D} \gamma_5] = \det \not{D}^\dagger \qquad \to \qquad \det \not{D} = (\det \not{D})^*$$

- one can also show $\det \not{D} > 0$
- thus, path integral weight is real and positive ✓

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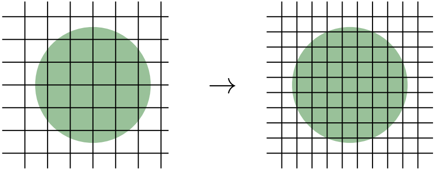
- one can also show $\det \not{D} > 0$
- thus, path integral weight is real and positive ✓
- same holds for staggered fermions with γ_5 replaced by $\eta_5 = (-1)^{n_1+n_2+n_3+n_4}$

Continuum limit

- continuum limit nonperturbatively



- lattice spacing from scale setting $\boxed{a(\beta)}$

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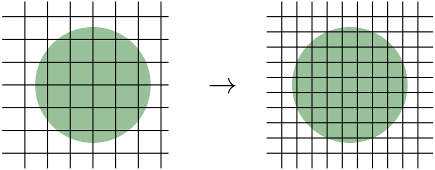

- lattice spacing from scale setting $\boxed{a(\beta)}$
- quark masses from line of constant physics $\boxed{m_f(\beta)}$

  tuned to the *physical point*:

  $M_\pi = 139$ MeV, $M_K = 495$ MeV, $M_p = 938$ MeV ...

Chiral symmetry and its breaking

- massless action $\bar{\psi} \not{D} \psi$ has chiral symmetry: $\{\gamma_5, \not{D}\} = 0$

$$\mathrm{SU}_V(N_f) \times \mathrm{SU}_A(N_f) \times \mathrm{U}_V(1) \times \mathrm{U}_A(1)$$

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  $\rightsquigarrow$ pseudo-Goldstone bosons: $N_f^2 - 1$ almost massless pions

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  $\rightsquigarrow$ pseudo-Goldstone bosons: $N_f^2 - 1$ almost massless pions
- high temperature: chiral symmetry restoration

Dictionary 2.

	Ising model	QCD
symmetry group	$\mathrm{Z}(2)$	$\mathrm{SU}(2)$
spontaneous breaking	$\langle M \rangle = \frac{\partial \log \mathcal{Z}}{\partial h}$	$\langle \bar{\psi}_u \psi_u \rangle = \frac{\partial \log \mathcal{Z}}{\partial m_u}$
Goldstones	–	3
explicit breaking	h	$m_u = m_d$
symmetry restoration	at high T	at high T

Chiral condensate

- full QCD expectation value

$$\langle\bar{\psi}_u\psi_u\rangle = \frac{T}{V}\frac{1}{\mathcal{Z}}\int \mathcal{D}U\,\mathcal{D}\bar{\psi}\,\mathcal{D}\psi\, e^{-\beta S_G-\bar{\psi}M\psi}\,\bar{\psi}_u\psi_u$$

$$= \frac{T}{V}\frac{1}{\mathcal{Z}}\int \mathcal{D}U\,\det M\, e^{-\beta S_G}\,\mathrm{tr}\,M_u^{-1} \qquad \leftarrow \text{way to calculate}$$

$$= \frac{T}{V}\frac{\partial \log \mathcal{Z}}{\partial m_u}$$

- remember order parameter definition for Ising model

$$\lim_{h\to 0^+}\lim_{V\to\infty}\langle M\rangle \qquad \text{or} \qquad \lim_{V\to\infty}\langle|M|\rangle_{h=0}$$

Chiral condensate

- full QCD expectation value

$$\begin{aligned}\langle\bar{\psi}_u\psi_u\rangle &= \frac{T}{V}\frac{1}{\mathcal{Z}}\int \mathcal{D}U\,\mathcal{D}\bar{\psi}\,\mathcal{D}\psi\, e^{-\beta S_G-\bar{\psi}M\psi}\,\bar{\psi}_u\psi_u \\ &= \frac{T}{V}\frac{1}{\mathcal{Z}}\int \mathcal{D}U\ \det M\, e^{-\beta S_G}\,\mathrm{tr}\, M_u^{-1} \qquad \leftarrow \text{way to calculate} \\ &= \frac{T}{V}\frac{\partial \log \mathcal{Z}}{\partial m_u}\end{aligned}$$

- remember order parameter definition for Ising model

$$\lim_{h\to 0^+}\lim_{V\to\infty}\langle M\rangle \qquad \text{or} \qquad \lim_{V\to\infty}\langle |M|\rangle_{h=0}$$

- here only option:

$$\lim_{m_u\to 0^+}\lim_{V\to\infty}\langle\bar{\psi}_u\psi_u\rangle$$

Renormalization

- remember UV divergences from free case (u and s flavors)

$$\log \mathcal{Z}_{\rm vac}^{\rm free} = \mathcal{O}(\Lambda^4) + \mathcal{O}((m_u^2+m_s^2)\Lambda^2) + \mathcal{O}((m_u^2+m_s^2)^2 \log \Lambda^2) + \text{finite}$$

  so the condensate

$$\langle \bar\psi_u \psi_u \rangle = \frac{\partial \log \mathcal{Z}_{\rm vac}^{\rm free}}{\partial m_u} = \mathcal{O}(m_u \Lambda^2) + \mathcal{O}(m_u(m_u^2+m_s^2)\log \Lambda^2) + \text{finite}$$

- multiplicative divergence (interacting case) Peskin, Schroeder

$$m_f^{\rm r} = Z_m \cdot m_f \qquad \forall\, f$$

- fully renormalized combination

$$\left[\langle \bar\psi_u \psi_u \rangle_T - \langle \bar\psi_u \psi_u \rangle_{T=0} \right] \cdot m_u$$

- sometimes also used

$$m_s \langle \bar\psi_u \psi_u \rangle_T - m_u \langle \bar\psi_s \psi_s \rangle_T$$

  cancels quadratic divergence but not the logarithmic one

Finite temperature transition in full QCD

Chiral restoration in full QCD

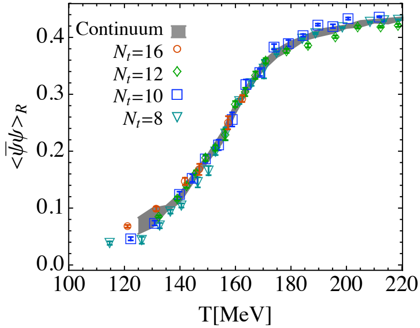
Results: condensate

- average light quark condensate after renormalization

$$\langle\bar{\psi}\psi\rangle^{\rm r} = -\left[\langle\bar{\psi}_u\psi_u\rangle_T - \langle\bar{\psi}_u\psi_u\rangle_{T=0}\right]\cdot\frac{m_u}{m_\pi^4}$$

watch out: this vanishes at $T = 0$ and positive at high T

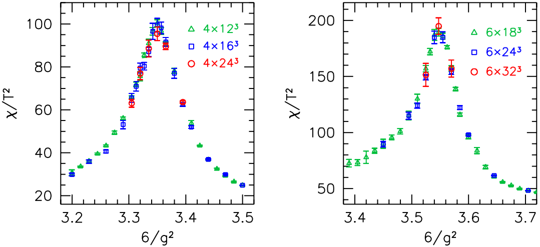
Borsányi et al. JHEP '10



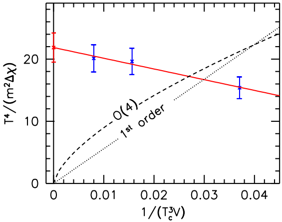
- does not look like a real phase transition. how to check?

Results: order of transition

- chiral susceptibility $\chi_{\bar{\psi}\psi}$ 🔗 Aoki, Endrődi et al. Nature '06



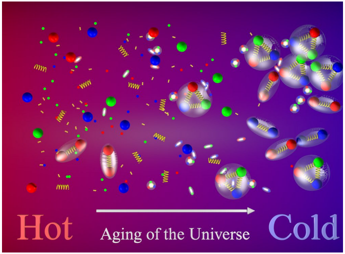
- volume scaling of peak height $\chi(V, T_c(V)) \propto L^0$



- confirmed by other discretizations 🔗 Bhattacharya et al. PRL '14

Crossover transition

- in full QCD at the physical point, there is no real phase transition but merely an analytic crossover

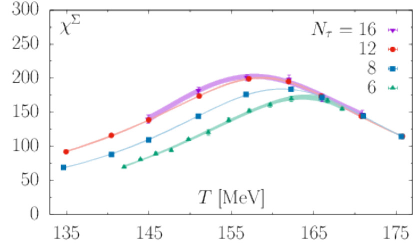


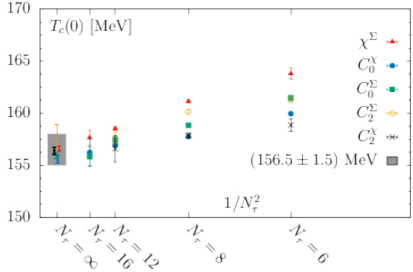
- there is no bubble formation in the QCD epoch of the early universe
  $\rightsquigarrow$ relevant for cosmology

Transition temperature

- at what temperature does the transition take place?
- there is no unique T_c but we can define it via
  - inflection point of $\langle\bar{\psi}\psi\rangle$
  - maximum of $\chi_{\bar{\psi}\psi}$
  - any characteristic behavior

🔗 Bazavov et al. PLB '19





- transition at $T_{pc} = 156.5(1.5)$ MeV
- transition width $\mathcal{O}(15)$ MeV

Deconfinement in full QCD

Center symmetry in full QCD

- remember center transformation

$$U_t(\mathbf{n}, \bar{n}_4) \to V_\zeta \cdot U_t(\mathbf{n}, \bar{n}_4) \quad V_\zeta \in \mathbb{Z}(3)$$

- gauge action is invariant
- det M in heavy-quark expansion:

$$\det M \propto \det\left(1 + \frac{\not{D}}{m}\right) = \exp\left[\operatorname{tr}\log\left(1 + \frac{\not{D}}{m}\right)\right] = \exp\left[-\sum_{k>0} \frac{\operatorname{tr}(\not{D}/m)^{2k}}{2k}\right]$$

  this includes Polyakov loop

- det M not invariant under center transformations
  it serves as explicit breaking for $\mathbb{Z}(3)$ symmetry

  which center sector does it prefer?

Center symmetry in full QCD

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

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

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 Dirac eigenvalues (Matsubara frequencies $n \in \mathbb{Z}$)

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

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

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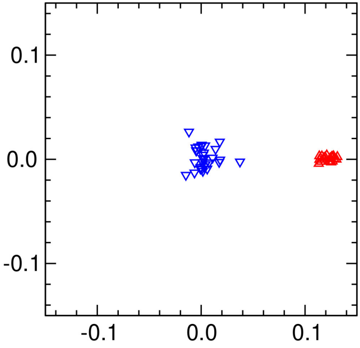
Polyakov loop in full QCD

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



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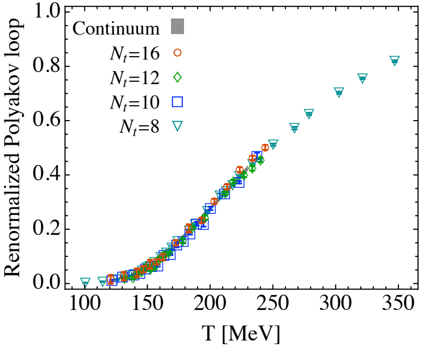
Goldstones	–	–	3
exp. breaking	$h > 0$	$m_u = m_d < \infty$	$m_u = m_d > 0$
symm. restoration	at high T	at low T	at high T

Results: Polyakov loop in full QCD

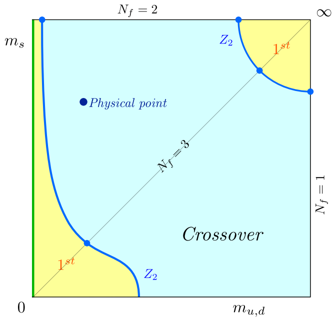
- fixed N_t-approach 🔗 Borsányi et al. JHEP '10



- 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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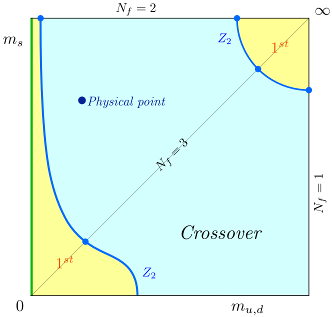

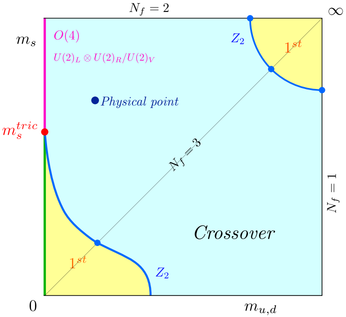

Cuteri et al. PRD '18

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

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

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

- 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

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

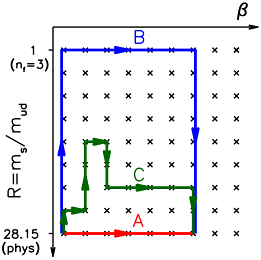
with starting point β_0 where $p^{\mathrm{r}}(T_0)/T_0^4 \approx 0$

- renormalized interaction measure

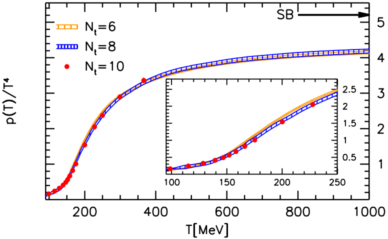
$$\frac{I^{\mathrm{r}}}{T^4} = \frac{N_t^3}{N_s^3}\frac{a(\beta)}{a'(\beta)} \left[\langle S_G\rangle_{N_s^3 N_t} - \langle S_G\rangle_{N_s^4} + \sum_f \left(\langle\bar\psi_f\psi_f\rangle_{N_s^3 N_t} - \langle\bar\psi_f\psi_f\rangle_{N_s^4} \right) \frac{\partial m_f}{\partial\beta} \right]$$

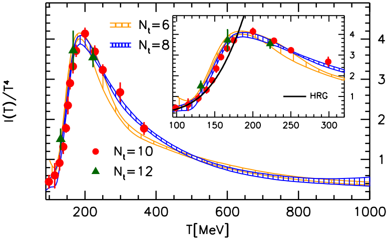
Integration paths

- integral is independent of integration path



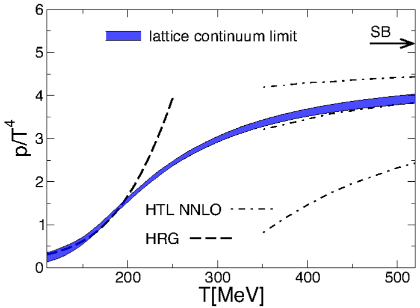
- averaging over different paths 🔗 Borsányi, Endrődi et al. JHEP '10

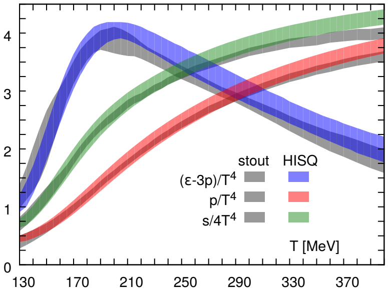




Results: equation of state

- 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

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

- 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

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

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

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

Chemical potential on the lattice

Chemical potential on the lattice

- add $\mu\gamma_4$ to naive 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

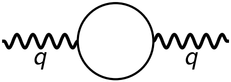
$$\log\det M_{\text{free}}(\mu) = \mathcal{O}(a^{-4}) + \mathcal{O}(m^2 a^{-2}) + \mathcal{O}(m^4 \log a) + \mathcal{O}(\mu^2 a^{-2})$$

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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- in the free case ($U_\mu = \mathbb{1}$) $\log\det M$ contains divergences
  Hasenfratz, Karsch PLB '83

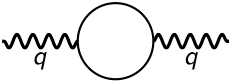
$$\log\det M_{\mathrm{free}}(\mu) = \mathcal{O}(a^{-4}) + \mathcal{O}(m^2 a^{-2}) + \mathcal{O}(m^4 \log a) + \mathcal{O}(\mu^2 a^{-2})$$

so the number density

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

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

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



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)

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

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

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

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

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forward/backward propagation enhanced/suppressed
links not unitary anymore

Sign problem

- remember η_5-hermiticity of staggered Dirac operator at $\mu = 0$
- now: $\{$forward hopping$\} \neq \{$backward hopping$\}^\dagger$

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

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

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

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- sign problem
- bonus staggered problem: ambiguous complex rooting

Sign problem - workarounds

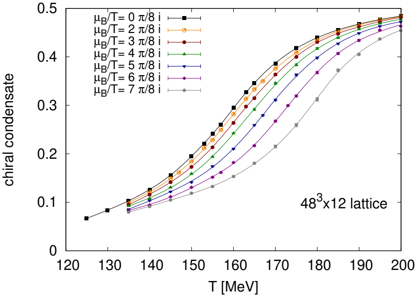
- here: brief description of
  - imaginary chemical potentials and analytical continuation
- many other approaches
  - reweighting
  - Taylor expansion in μ around $\mu = 0$
  - complex Langevin
  - Lefschetz thimbles
  - ...

Analytic continuation from imaginary μ

- again {forward hopping} = {backward hopping}†

$$\eta_5 \not{D}(i\theta)\eta_5 = \not{D}^\dagger(i\theta)$$

- so standard simulations work at $\theta \neq 0$ $(\mu^2 < 0)$ Borsányi et al. PRL '20



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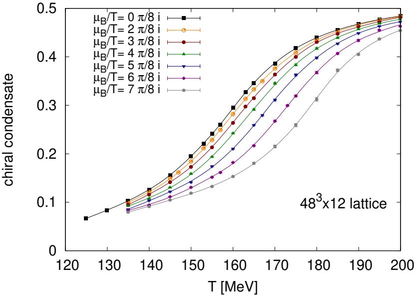
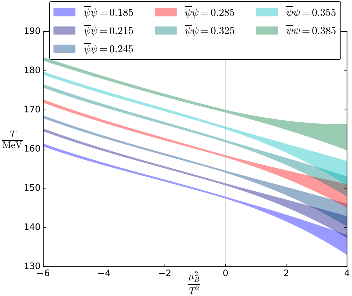


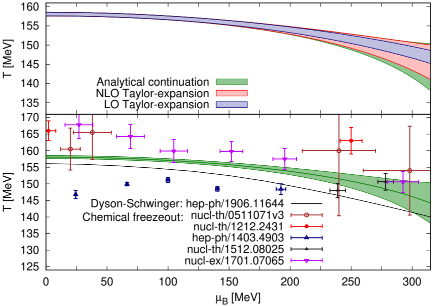


- fit and analytically continue to $\mu^2 > 0$

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:

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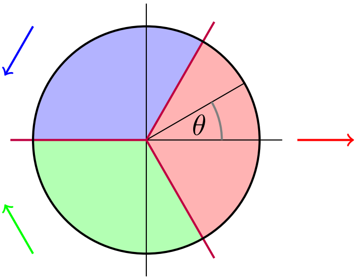
- magnitude of lowest frequency is largest for:

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

Roberge-Weiss transitions

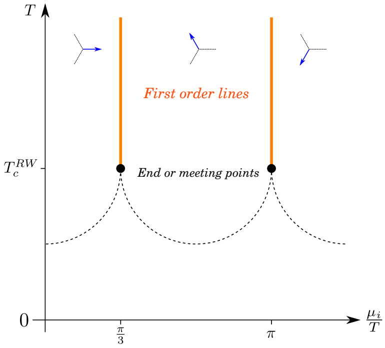
- preferred center sectors at nonzero θ



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

Summary

Summary

- lattice QCD is a first-principles approach to study elementary particles and also a lot of fun
- inputs
  - QCD Lagrangian
  - 1 quantity to set lattice scale $a(\beta)$
  - N_f quantities to set bare quark masses $m_f(\beta)$
- research on QCD thermodynamics
  - at physical quark masses at zero density: ✓
  - in the massless limit: ongoing
  - at physical quark masses at $\mu/T \lesssim 1$: ✓
  - large densities: ×
  - background magnetic fields: ✓
  - isospin density: ✓
- more on that at XQCD 2022 in Trondheim