QCD thermodynamics on the lattice

Attila Pásztor

ELTE Eötvös Loránd University, Budapest

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Why study $T > 0$ QFT on the lattice?

Approximately thermal systems

- Cosmological history
- Supernovae, neutron star inspirals
- Heavy ion collision

Non-perturbative phenomena

- Near the QCD transition
- No clear separation of scales $T \approx gT \approx g^2 T \approx \Lambda_{QCD} \approx 1.0/(R_{\mathrm{instanton}})$
- There are also non-perturbative phenomena even at weak coupling

Interesting

- A number of well defined problems that remain unsolved
- Connections with many fields and methods of physics (stat mech, condensed matter theory, EFTs, cosmology, heavy ion physics etc.)

1. Phase transitions and finite-size scaling
2. Lattice field theory
3. Deconfinement in pure gauge theory
4. The QCD crossover transition
5. The chemical potential
6. Taylor series in μ
7. Imaginary chemical potential
8. Reweighting

Finite-size scaling - away from transitions

Away from phase transitions
The free energy density $f_L \equiv F_L/L^3$ has an infinite volume limit.
With open boundary conditions:

$$f_\infty - f_L \sim -f_S \frac{1}{L}$$

With periodic boundary conditions:

$$f_\infty - f_L \sim e^{-\Gamma L}$$

E.g., in QCD: $T \ll T_c$

$$f_\infty - f_L \sim e^{-m_\pi L}$$

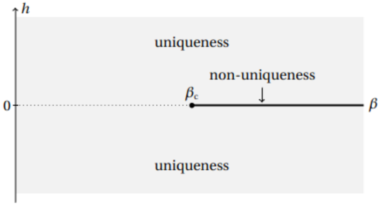
- Asymptotics determined by $L = \infty$ properties of the theory.
- $f(L) \sim g(L)$ means $\lim_{L\to\infty} \frac{\log f(L)}{\log g(L)} = 1$

The phase diagram of the Ising model in $d \geq 2$

$$Z = \sum_{\{s_i\}} e^{\beta \sum_{\langle ij \rangle} s_i s_j + h \sum_i s_i}$$

$$\langle s \rangle = \frac{1}{L^d} \langle M \rangle = \frac{1}{L^d} \frac{\partial \log Z}{\partial h}$$

$$\chi = \frac{1}{L^d}(\langle M^2 \rangle - \langle M \rangle^2) = \frac{1}{L^d} \frac{\partial^2 \log Z}{\partial h^2}$$



1st order phase transition: non-unique infinite volume limit

- Different boundary conditions $\rightarrow$ different inf. vol. lim.
- With fixed boundary conditions (say periodic):

$$\lim_{N \to \infty} \lim_{h \to 0^+} \langle s \rangle = 0 \neq \lim_{h \to 0^+} \lim_{N \to \infty} \langle s \rangle = M_S$$

1st order transitions

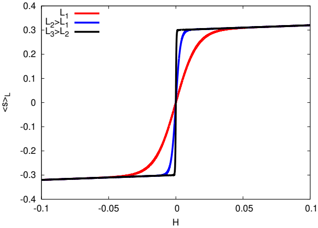
1st order transition: **coexistence**

Finite-size scaling at 1st order transitions

1st order transition: **coexistence**

Model the probability distribution of the order parameter:

$$P(s) = \sqrt{\frac{L^d}{2\pi\chi_T}} \times \left(\frac{e^{HM_S L^d}}{e^{HM_S L^d} + e^{-HM_S L^d}} \exp\left[-\frac{(s - M_S - \chi_T H)^2 L^d}{2\chi_T}\right] + \frac{e^{-HM_S L^d}}{e^{HM_S L^d} + e^{-HM_S L^d}} \exp\left[-\frac{(s + M_S - \chi_T H)^2 L^d}{2\chi_T}\right] \right)$$



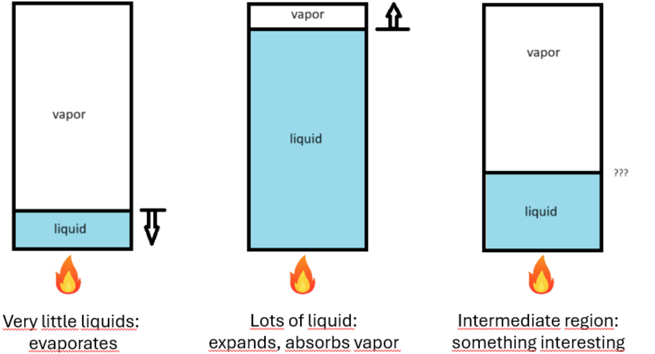
$$\langle s \rangle_L = \chi_T H + M_S \tanh(HM_S L^d)$$

$$\chi = \frac{\partial \langle s \rangle_L}{\partial H} = \chi_T + \frac{M_S^2 L^d}{\cosh^2(HM_S L^d)}$$

width $\sim L^{-d}$ height $\sim L^d$

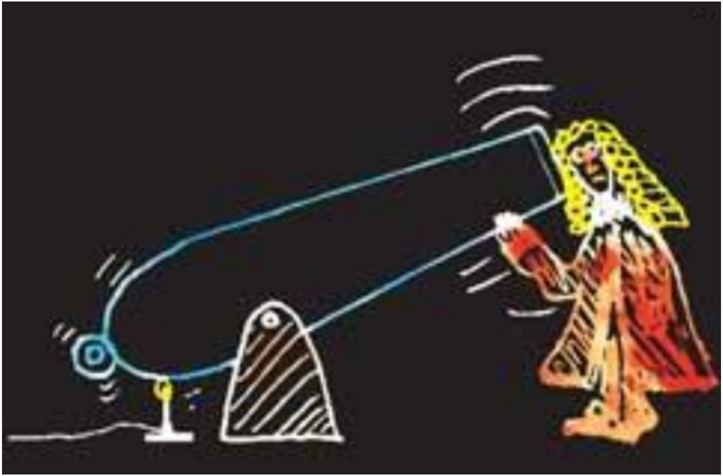
What happens when we heat water in a closed container?

Charles Cagniard de la Tour, 1822 $\rightarrow$ discovery of the critical point



At the critical point (2nd order transition): $\rho_{liquid} = \rho_{vapor}$

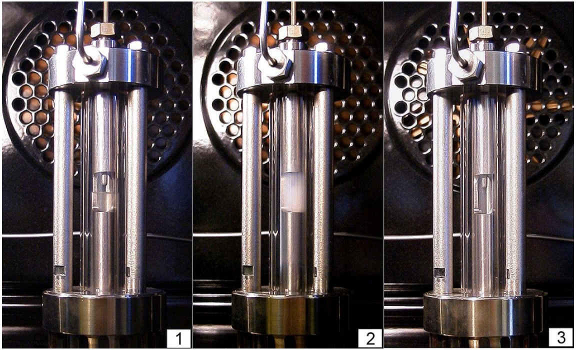
Charles Cagniard de la Tour, 1822



https://edu.rsc.org/feature/supercritical-processing/2020235.article

2nd order transitions

2nd order transition: **diverging correlation length**



HEATING $\longrightarrow$

size of density fluctuations $\sim \lambda_{light} \rightarrow$ critical opalescence

Finite-size scaling - 2nd order transitions

- Second order transition: **diverging correlation length**
- Infinite volume:

$$\xi \sim |t|^{-\nu} \qquad \chi \sim |t|^{-\gamma} \qquad t = (T - T_c)/T_c$$
$$\rightarrow \chi \sim \xi^{\gamma/\nu}$$

- If ξ diverges, it will not fit in the box $\xi \rightarrow L$:

$$\chi \sim L^{\gamma/\nu}$$

- 3D Ising: $\gamma \approx 1.24 \qquad \nu \approx 0.63 \rightarrow \gamma/\nu \approx 1.96 < d = 3$
- Rule of thumb:

$$\langle O \rangle_{L=\infty}(t) \sim t^{-\rho} \qquad \rightarrow \qquad \langle O \rangle_{T=T_c}(L) \sim L^{\rho/\nu}$$

Finally, crossovers

Crossovers

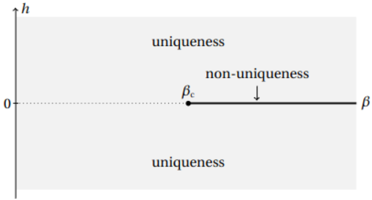
- Close to a critical point, but not quite there (e.g. residual field h_0)
- Correlation length ξ large, but finite
- For $L \ll \xi$ behaves like a critical system
- For $L \gg \xi$ hehaves like a system away from criticality

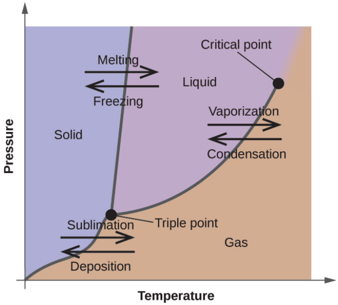
Summary
Susceptibility (variance) of the order parameter: $\chi(L, T = T_c) \sim L^k$

k	transition type
0	crossover
γ/ν	2nd order
d	1st order

Universality classes and non-universal maps

- Types of d.o.f. (scalar, vector, tensor); symmetries; spatial dimensions; interaction range determine the critical exponents and the singular part of the free energy near 2nd order transitions
- The mapping of the variables in the different models is not universal





Good textbooks covering finite-size scaling and criticality in more detail:
Goldenfeld; Binder & Heermann; M.N. Barber in Domb, Lebowitz Vol. 8.;

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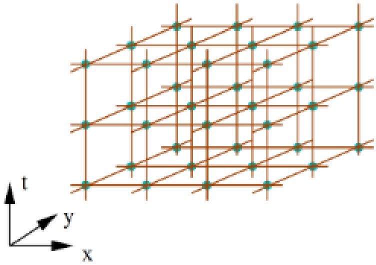
The lattice regularization



- Integral over spacetime $\int d^4x(\dots) \to$ sum over sites $a^4 \sum_x (\dots)$
- Derivatives $\partial_\mu \phi \to$ finite differences $\frac{1}{a}\left(\phi(x+\hat{\mu}) - \phi(x)\right)$
- $\phi \Box \phi \to$ hopping $\frac{1}{a^2} \sum_\mu \left(\phi(x-\hat{\mu})\phi(x) + \phi(x+\hat{\mu})\phi(x) - 2\phi(x)^2\right)$
- Momenta: $|p| \leq \pi/a$ natural cut-off (Brillouin zone)
- Renormalization needed to make certain quantities finite as $a \to 0$
- Cut-off effects: $\langle O \rangle_{lattice} = \langle O \rangle_{continuum} + O(a^\nu)$
- To get physical results, we need to perform:
  - Continuum limit: $a \to 0$
  - Infinite volume (thermodynamic) limit: $L[\text{fm}] \to \infty$

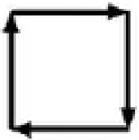
Gauge symmetry and parallel transport

- Take N-component scalar (Dirac also works): $\phi(x)(\Box + m^2)\phi(x)$.
- It has a global symmetry: $\phi(x) \to \Lambda^{-1}\phi(x)$ where $\Lambda \in SU(3)$
- We want to make it local $\Lambda \to \Lambda(x)$
- Then $\phi(x)$ and $\phi(y)$ transform with a different matrix
- We introduce a parallel transporter $U(\mathcal{C}_{x\to y})$:

$$U(\mathcal{C}_{x\to y}) \to \Lambda(y)^{-1} U(\mathcal{C}_{x\to y})\Lambda(x)$$

- Now $U(\mathcal{C}_{x\to y})\phi(x)$ transforms with $\Lambda(y)$
- Continuum FT: $U(\mathcal{C}_{x\to x+dx}) = \mathbf{1} - A_\mu dx^\mu$ (Lie-algebra valued)
- Lattice FT: we use the parallel transporters (Lie-group valued)
- Exact gauge symmetry at finite lattice spacing (Renormalization!)
- Covariant derivatives: add parallel transporter to hopping terms
- Dynamics for the gauge fields: (traces of) closed loops in the action
- Gauge invariant observables: polynomials of $\phi(x)$, $\phi(x)U(\mathcal{C}_{x\to y})\phi(y)$, $Tr(U(\mathcal{C}_{\text{closed loop}}))$

The plaquette action



- The simplest close loop is a 1X1 square.
- This gives the Wilson (or plaquette) gauge action.

$$S_P = \frac{1}{2}\sum_x \sum_{\mu\nu} \beta \left(1 - \frac{1}{N}\,\mathrm{Re}\,\mathrm{Tr}\, U_{x,\mu\nu}\right) = \frac{-\beta}{4N}\sum_x \sum_{\mu\nu} a^4\,\mathrm{Tr}\,(F_{\mu\nu}F_{\mu\nu}) + O(a^6)$$

- The bare gauge coupling: $\beta = 2N/g^2$
- Also need $SU(3)$ invariant integral measure to define path path integral (Haar-measure)

The continuum limit

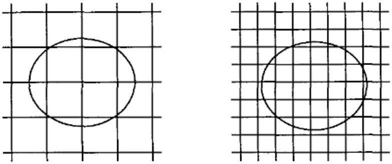


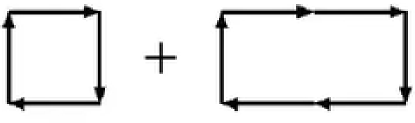
Fig. 9-1 Making the lattice finer by tuning the coupling with the lattice spacing so as to keep physics the same.

- Correlation function: $\left\langle \phi(\vec{0},\tau)\phi(\vec{0},0) \right\rangle \sim e^{-(m_\phi a)(\tau/a)} = e^{-(\tau/a)/(\xi/a)}$
- $m/\mathrm{MeV} = \text{fixed},\ a \to 0 \leftrightarrow \xi/a \to \infty$: 2nd order transition (RG FP) in the lattice thy
- For non-abelian gauge thy, the FP is Gaussian (asymptotic freedom)
- In many parameter theories: line of constant physics: change bare parameters such that IR quantities (e.g. mass ratios) are fixed while $a \to 0$, this def. how one has to approach the FP

Symanzik improvement

- RG theory tells us that we can add irrelevant operators to the action without changing the continuum limit.
- But the cut-off effects will be different
- By a clever choice of the irrelevant operators, they can be made smaller
- Systematic (perturbative) approach: Symanzik

For pure gauge theory, just adding a 2X1 rectangular loop with a well chosen coefficient improves cut-off effects drastically:



Finite temperature

- Euclidean time: $e^{iHt} = e^{-H\tau}$ and $e^{iS[\phi]} \to e^{-S_E[\phi]}$
- Path integral: periodic/antiperiodic BCs for bosons/fermions:
  - Bosonic frequencies: $\omega_n = 2n\pi T$ (PBC in time)
  - Fermionic frequencies: $\omega_n = (2n+1)\pi T$ (APBC in time)
- On the lattice:

$$T = \frac{1}{N_\tau a}$$

- For fixed T, the continuum limit is taken by taking $N_\tau \to \infty$

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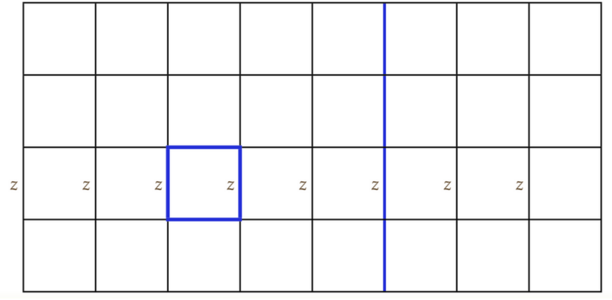
Center symmetry and the Polyakov loop

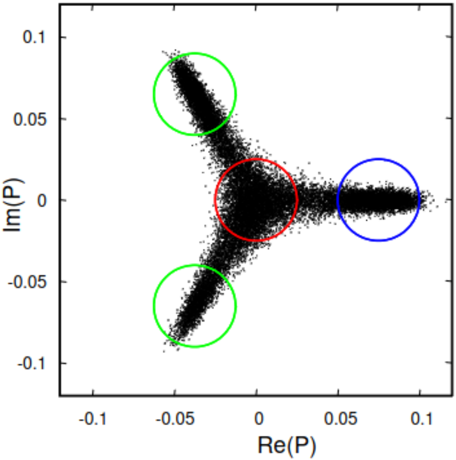


- Multiply links in a time slice with $z^k = \exp\left(\frac{2\pi i k}{N}\right)$
- Center: commutes with all $SU(3)$ group elements
- Action and integral measure (is invariant, but the Polyakov loop is not:

$$P_x = \frac{1}{N} \operatorname{Tr} \left(\prod_{\tau=0}^{N_\tau - 1} U_4(\tau, x) \right) \to z^k P_x$$

- Order parameter for SSB of center symmetry
- Related to confinement: $\langle P \rangle = e^{-F_Q/T} \leftrightarrow \langle P \rangle = 0 \leftrightarrow F_Q = \infty$

Scatter plot of the Polyakov loop near β_c



Confined: red; Deconfined real: blue; Deconfined complex: green

A small $1/m$: favors the blue sector

Plot from 2112.05454

What happens to center symmetry with quarks?

- Fix temporal gauge $U_{x4} = 1$ ($A_{x4} = 0$). You can do this for all, but the last timeslice, where the (untraced) Polyakov loops remain.
- Further fix the Polyakov gauge, by diagonalizing the Polyakov loops: $P = diag(e^{i\phi_1}, e^{i\phi_2}, e^{-i(\phi_1+\phi_2)})$
- In pure gauge theory we had three Polyakov sectors at:

$$\phi_1 \approx \phi_2 \approx 0 \quad \phi_1 \approx \phi_2 \approx 2\pi/3 \quad \phi_1 \approx \phi_2 = -2\pi/3$$

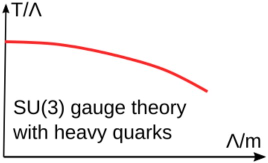
- In a theory with fermions this change in the boundary conditions shifts the Matsubara frequencies to:

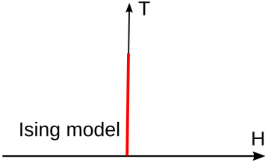
$$(2n + 1 + 0)\pi T \quad (2n + 1 + 2/3)\pi T \quad (2n + 1 - 2/3)\pi T$$

- The magnitude of the lowest frequency (and so the quark determinant) is largest for $\phi_1 \approx \phi_2 \approx 0$.

Symmetry breaking pattern for QCD with heavy quarks

	SU(3) gauge theory	Ising model
symmetry	Z_3	Z_2
order parameter	$\langle P \rangle$	$\langle s \rangle$
explicit breaking	$1/m$	h
symmetry restoration	low T	high T



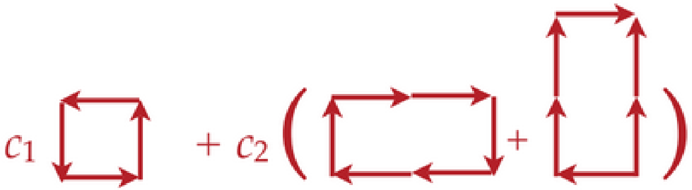


Ongoing research: locating the heavy critical mass
The critical mass is very large ($m_\pi \sim O(5GeV)$)!
The deconfinement transition in $SU(3)$ gauge theory is a weak first order

Simulating pure pure SU(3) gauge theory on the lattice

For concreteness, use the tree-level Symanzik improved gauge action

$$S_G = \frac{\beta}{N} \sum_x \sum_{\mu<\nu} \left(1 - \mathrm{Re}\,\mathrm{Tr}\left(c_1 P_{x,\mu\nu} + c_2(R^1_{x,\mu\nu} + R^2_{x,\mu\nu})\right)\right)$$

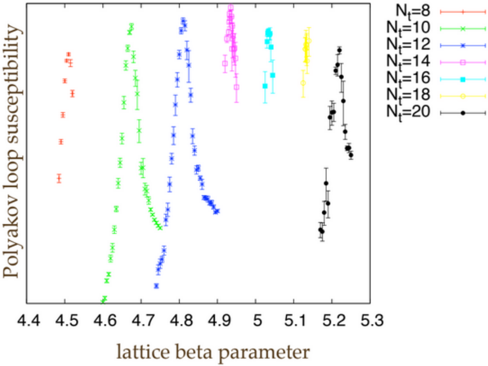


- The plaquette action has $O(a^2)$ error
- By adding 2x1 rectangles, the $O(a^2)$ errors can be removed with $c_1 = 5/3$ and $c_2 = -1/12$ (tree-level/classical improvement)
- In the interacting theory, however, $O(g^2 a^2)$ errors appear

$\beta_c(N_\tau)$ for pure glue

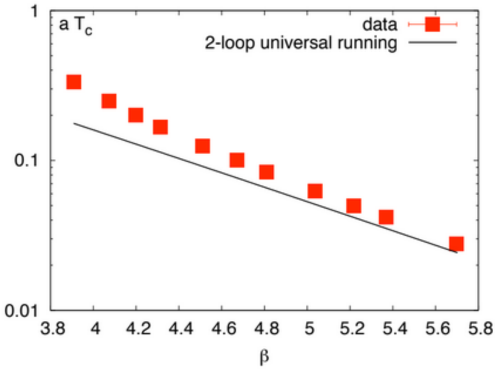
Nt	βc
3	3.90812(7)
4	4.07252(13)
5	4.19963(14)
6	4.31466(24)
8	4.5092(27)
10	4.6729(75)
12	4.811(10)
16	5.037(16)
20	5.217(30)
24	5.3690(27)
36	5.6985(42)

tree-level Symanzik action



- For a transition in the continuum QFT, β_c should increase with N_t.
- This is in contrast with a bulk transition

The lattice spacing and T_c



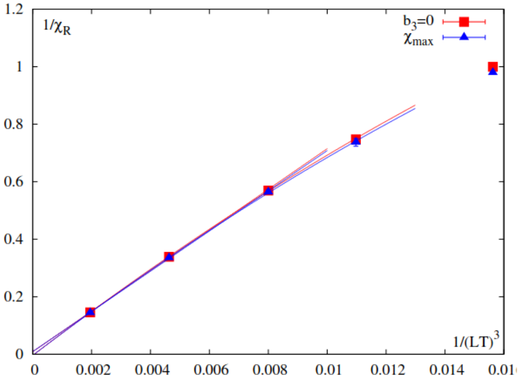
$aT_c = 1/N_t$, compare with two-loop universal result:

$$(\Lambda a)(\beta) = \left(\frac{\beta}{2Nb_0}\right)^{b_1/2b_0^2} \exp\left(-\frac{\beta}{4Nb_0}\right) \qquad b_0 = \frac{11N}{16\pi^2} \qquad b_1 = \frac{34}{3}\left(\frac{N}{16\pi^2}\right)^2$$

In fact $T_c/\Lambda = 1.26(7)$

Finite volume scaling

- Renormalize the susceptibility
- Continuum extrapolate at fixed volumes
- Perform finite volume scaling in the continuum theory
- $\chi^{-1} \sim V^{-1}$ with a small subleading correction



Plot from Borsányi et al, Phys.Rev.D 105 (2022) 7, 074513

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Chiral symmetry

- massless Dirac operator has chiral symmetry $\{D\gamma_5\} = 0$

$$SU(N_f)_L \times SU(N_f)_R \times U(1)_V \times U(1)_A$$

- Spontaneously broken:

$$SU(N_f)_L \times SU(N_f)_R \to SU(N_f)_V$$

  $\to$ Goldstone bosons: $N_f^2 - 1$ massless pions
- Axial symetries also explicitly broken by quark masses
  $\to$ pseudo-Goldstone bosons: $N_f^2 - 1$ light pions
- High-temperature: chiral symmetry restoration
- $U(1)_A$ also broken by the anomaly

QCD symmetry breaking pattern

	QCD		Ising model
spontaneous breaking	$Z_3 \to \emptyset$	$SU(N_f)_L \times SU(N_f)_R \to SU(N_f)_V$	$Z_2 \to \emptyset$
order parameter	$\langle P \rangle$	$\left\langle \bar{\psi}\psi \right\rangle$	$\langle s \rangle$
Goldstone bosons	-	$N_f^2 - 1$	-
explicit breaking	$1/m$	m	h
symmetry restoration	low T	high T	high T

I swept the anomaly under the rug, for now.

Lattice fermions on one slide

$$Z = \int \mathcal{D}U\mathcal{D}\psi\mathcal{D}\bar{\psi} e^{-S_{YM}(U) - \bar{\psi}(D+m)\psi} = \int \mathcal{D}U \det(D+m) e^{-S_{YM}(U)}$$

Nielsen-Ninomiya theorem
Impossible for a massless lattice Dirac operator D to satisfy all of:

1. Correct continuum limit: $G^{-1}(p) \sim i\gamma_\mu p_\mu$ as $a \to 0$
2. Locality: $G^{-1}(p)$ a continuous function of p
3. Continuum chiral symmetry: $\{D\gamma_5\} = 0$
4. No doublers: Describes only one flavour in the continuum limit (one pole)

Compomises, compromises, ...

- **Wilson fermions:** $N_f = 1$, but $\{D\gamma_5\} \neq 0$:
  Additive mass renormalization (fine tuning), $O(a)$ cut-off effects
- **Staggered fermions:** $\{D\gamma_5\} = 0$ but $N_f = 4$:
  Staggered rooting $Z = \int \mathcal{D}U \det M(m,\mu,U)^{N_f/4} e^{-S_{YM}(U)}$
- **Ginsparg-Wilson/chiral/overlap fermions:** $N_f = 1$:
  Ginsparg-Wilson relation: $\{D\gamma_5\} = aD\gamma_5 D$, very expensive

Tuning

- In $N_f = 2 + 1$, in the simplest case (say staggered) we have three bare parameters: β controls the continuum limit, the quark masses have to be tuned to their physical values.
- This requires $T = 0$ simulations. One way to do it:
  1. Fix β
  2. Simulate at some m_u, m_s
  3. Measure $m_\pi a, m_K a, m_\Omega a$
  4. Use χPT formulae to guess where you should have simulated to have $m_\pi / m_\Omega = 135/1672$ and $m_K / m_\Omega = 495/1672$
  5. If you have not bracketed the physical point yet, GO TO 2)
  6. Once you have bracketed the physical point, interpolate
  7. Measure m_Ω, your lattice spacing is $a = (am_\Omega)_{LAT}/1672MeV$
- Doing this at several value of β gives $m_u(\beta)$, $m_s(\beta)$ and $a(\beta)$. Now you are ready to do the finite temperature simulations.

Finite temperature runs

- Spatial size $L = N_s a(\beta)$
- Temperature $T = 1/(N_t a(\beta))$
- Fixed-β approach: change T by changing N_t
  - Only discrete temperatures are possible ✗
  - Less $T = 0$ runs needed for tuning ✓
  - More common with Wilson fermions
- Fixed-T approach: chabge T by changing β
  - Continuous temperatures are possible ✓
  - More $T = 0$ runs needed ✗
  - More common with staggered fermions

Chiral observables for finite quark mass

Chiral condensate

$$\left\langle\bar{\psi}\psi\right\rangle_q = \frac{T}{V}\frac{\partial \log \mathcal{Z}}{\partial m_q}$$

Divergence structure:

- multiplicative (quark mass is renormalized multiplicatively)
- additive ($\sim m/a^2 + m^3 \log(a)$)

The multiplicative renormalization of the quark mass $m_r = Z_m m$ drops out from: $m_r \frac{\partial}{\partial m_r} = m \frac{\partial}{\partial m}$. $\rightarrow$ This combination is UV finite:

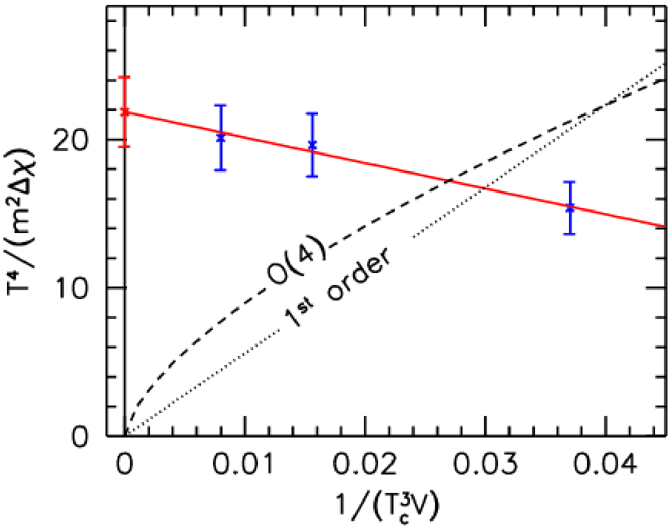
$$\left\langle\bar{\psi}\psi\right\rangle^R = -\left[\left\langle\bar{\psi}\psi\right\rangle_T - \left\langle\bar{\psi}\psi\right\rangle_0\right]\frac{m_{ud}}{f_\pi^4}$$

Chiral susceptibility

$$\chi_{\bar{\psi}\psi} = \frac{T}{V}\frac{\partial^2 \log \mathcal{Z}}{\partial m_q^2}$$

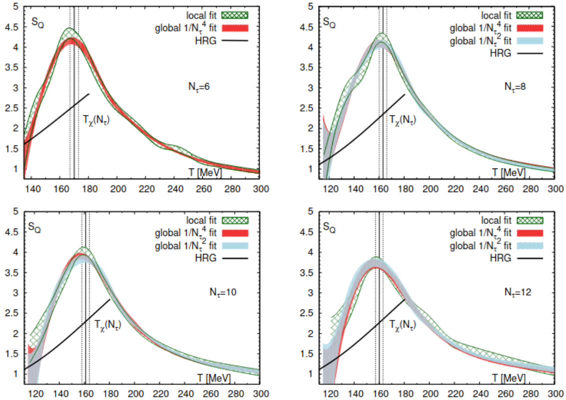
$$\chi_{\bar{\psi}\psi}^R = \left[\chi_T^{\bar{\psi}\psi} - \chi_0^{\bar{\psi}\psi}\right]\frac{m_{ud}^2}{f_\pi^4}$$

The chiral crossover for physical quark masses



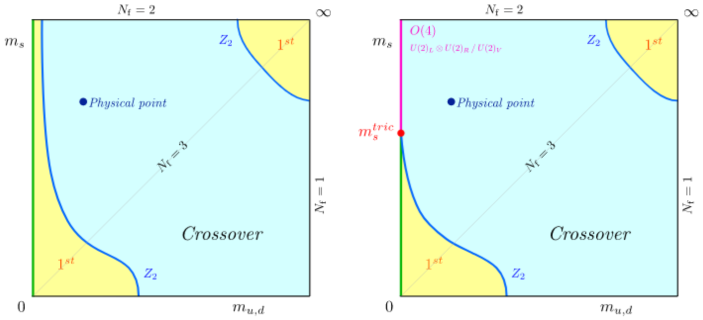
Wuppertal-Budapest: Nature 2006

Chiral vs deconfinement



- Inflection point of the Polyakov loop: scheme dependent
- Peak position of the static quark entropy is not $S_Q = -\frac{dF_Q}{dT}$
- Matches the T_c from chiral observables (Bazavov et al, PRD93, 2016)

Unsolved questions about the chiral limit (Columbia plot)



Plot from Cuteri et al, JHEP11(2021)141

- Perturbative RG (ϵ expansion) (Pisarski & Wilczek, 1984)
    - If anomaly recovered at T_c: $N_f = 2, 3$ cannot be 2nd order
    - If anomaly is present: $N_f = 2$ can be second order, $N_f = 3$ cannot
- If correct, then left: phase diagram without anomaly, right: with anomaly
- But pert. RG is not always reliable (see e.g. in 2201.07909)

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The grand canonical ensemble

$$\mathcal{Z} = \mathrm{Tr}\left(e^{-\left(H - \sum_i \mu_i N_i\right)/T}\right)$$

$$\langle O \rangle = \frac{1}{Z}\,\mathrm{Tr}\left(O e^{-\left(H - \sum_i \mu_i N_i\right)/T}\right)$$

- H : Hamiltonian
- N_i : conserved quantum numbers: $[H, N_i] = 0$
  E.g. in QCD: N_u,N_d,N_s or equivalently N_B, N_S, N_Q:
  $$\mu_u = \frac{1}{3}\mu_B + \frac{2}{3}\mu_Q \quad \mu_d = \frac{1}{3}\mu_B - \frac{1}{3}\mu_Q \quad \mu_s = \frac{1}{3}\mu_B - \frac{1}{3}\mu_Q - \mu_S$$
- T : temperature
- μ_i : chemical potentials

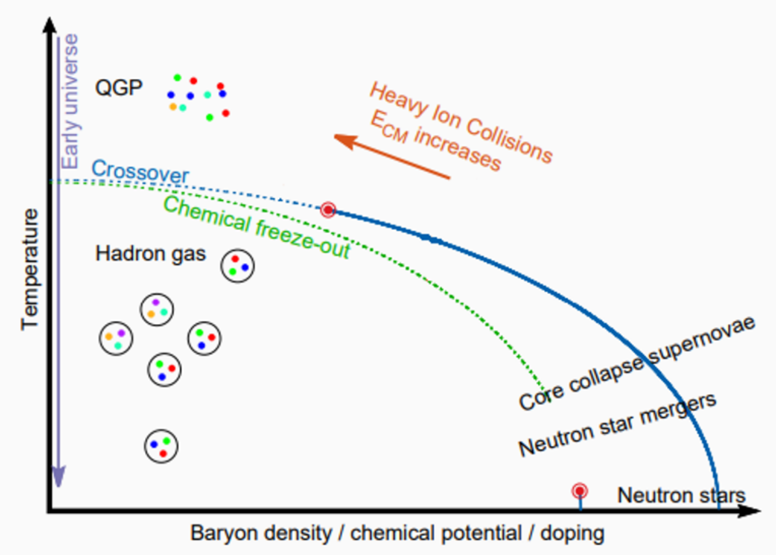
Some quantities follow by differentiation (Nice: no renormalization needed):

$$\chi_1^i = \frac{1}{T^3}\langle n_i \rangle = \frac{1}{VT^3}\frac{\partial \log \mathcal{Z}}{\partial \mu_i}$$

$$\chi_2^i = T\frac{\partial \langle n_i \rangle}{\partial \mu_i} = \frac{1}{V}\left(\left\langle N_i^2 \right\rangle - \langle N_i \rangle^2\right) \qquad = \frac{T^2}{V}\frac{\partial^2 \log \mathcal{Z}}{\partial \mu_i^2}$$

$$\chi_{11}^{ij} = T\frac{\partial \langle n_i \rangle}{\partial \mu_j} = \frac{1}{V}\left(\langle N_i N_j \rangle - \langle N_i \rangle \langle N_j \rangle\right) \quad = \frac{T^2}{V}\frac{\partial^2 \log \mathcal{Z}}{\partial \mu_i \partial \mu_j}$$

Conjectured phase diagram in the $T - \mu_B$ plane



Chemical potential: $A_0 = -i\mu$

Non-interacting fermions:

$$S_E(\mu = 0) = \int_0^{1/T} \int d^3x \bar{\psi}(\gamma_\nu \partial_\nu + m)\psi$$

Global symmetry: $\psi \to e^{i\alpha}\psi$, $\bar{\psi} \to \bar{\psi}e^{-i\alpha}$
Conserved charge (fermion number)

$$N = \int d^3x \bar{\psi}\gamma_0\psi$$

The weights we have to add to the path integral are $e^{\frac{\mu}{T}N}$, so:

$$S_E(\mu) = \int_0^{1/T} d\tau \int d^3x \bar{\psi}(\gamma_\nu \partial_\nu + \gamma_0\mu + m)\psi$$

The chemical potential is like a **constant imaginary Abelian gauge field in the Euclidean time direction** $A_0 = -i\mu$:

$$S_E(\mu) = \int_0^{1/T} \int d^3x \bar{\psi}(\gamma_\nu(\partial_\nu + iA_\nu) + \gamma_0\mu + m)\psi$$

In a $U(1)$ gauge theory ($N_f = 1$) μ can be removed by redefining A_0

Chemical potential: γ_5 hermiticity

Continuum Dirac operator:

$$M(\mu) = (\gamma_\nu(\partial_\nu + iA_\nu) + \gamma_0\mu + m)$$

At zero chemical potential:

$$\gamma_5 M(\mu = 0)\gamma_5 = M(\mu = 0)^\dagger$$
$$\det(\gamma_5 M \gamma_5) = \det M = \det(M^\dagger) = (\det M)^*$$

This was continuum, but versions of this also hold for lattice fermions For non-zero chemical potential:

$$\gamma_5 M(\mu)\gamma_5 = M(-\mu^*)^\dagger$$

$\rightarrow$ Complex action problem

- Purely imaginary chemical potential has no complex action problem
- Isospin chemical potential has no complex action problem: $|\det M(\mu)|^2 = \det M(\mu) \det M(-\mu)$

Chemical potential: lattice fermions

Naive: $\mu\bar{\psi}\gamma_0\psi \to$ UV divergent

Problem 1: does not couple to the exact conserved charge at a finite *a*
Problem 2: this is like a photon mass renormalization in QED (zero momentum) with a gauge symmetry breaking regulator
Hasenfratz, Karsch 1983

Both problems are solved by introducing the chemical potential as an imaginary Abelian gauge field in the time direction:

$$U_{x4} \to e^{\mu a} U_{x4} \qquad U^{\dagger}_{x4} \to e^{-\mu a} U^{\dagger}_{x4}$$

Chemical potential as boundary condition

One way to see it:

- Expand the gluonic effective action $S_{YM} - \ln\det(D+m)$ in loops
- Forward hops in time: weight with $e^{\mu a}$; backward: $e^{-\mu a}$
- For any loop that does not wrap around the time direction: 1
- For any loop that wraps around the time direction: $e^{\mu a N_\tau N_{wrap}}$
- We might as well put the chemical potential on a timeslice (say the last) as $e^{\mu/T}$ and get the same

Another way to see it:

- Use the field redefinition: $\psi_x = e^{-\mu\tau}\psi_x'$ and $\bar\psi_x = e^{+\mu\tau}\bar\psi_x'$
- The μ dependence then drops for all terms $\bar\psi_x e^{\mu}\psi_{x+4}$ and $\bar\psi_{x+4}e^{-\mu}\psi_x$ and becomes a boundary condition:

$$\psi_{N_\tau}' = -e^{\mu/T}\psi_0'$$

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The Taylor method

$$\mathcal{Z} = \int \mathcal{D}U \det M_u(U, m_u, \mu_u) \det M_d(U, m_d, \mu_d) \det M_s(U, m_s, \mu_s) e^{-S_G(U)}$$

Now calculate derivatives at $\mu = 0$, e.g.:

$$\chi_2^u = \frac{1}{VT^2} \frac{\partial^2 \log \mathcal{Z}}{\partial^2 \mu_u} = \frac{1}{VT^2} \left\langle B_u + A_u^2 \right\rangle$$

$$\chi_{11}^{ud} = \frac{1}{VT} \frac{\partial^2 \log \mathcal{Z}}{\partial \mu_u \partial \mu_d} = \frac{1}{VT} \left\langle A_u A_d \right\rangle$$

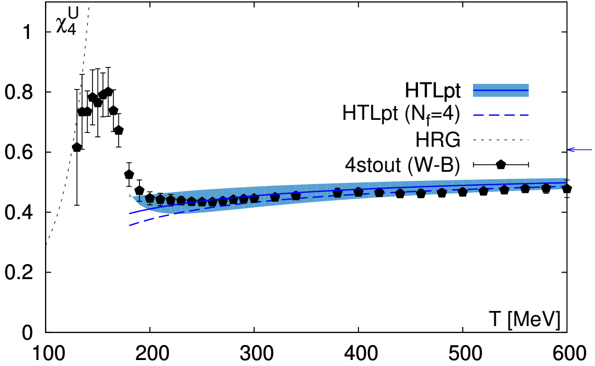
$$A_u = \frac{\partial}{\partial \mu_u} \ln \det M_u = \mathrm{Tr} \left(\frac{\partial M_u}{\partial \mu_u} M_u^{-1} \right)$$

$$B_u = \frac{\partial^2}{\partial \mu_u^2} \ln \det M_u = \; Tr \left(\frac{\partial M_u}{\partial \mu_u} M_u^{-1} - M_u^{-1} \frac{\partial^2 M_u}{\partial \mu_u^2} M_u^{-1} \frac{\partial M_u}{\partial \mu_u} \right)$$

Higher derivatives and derivatives of other observables from:

$$\frac{\partial}{\partial \mu_i} \left\langle X \right\rangle = \left\langle \frac{\partial}{\partial \mu_i} X \right\rangle + \left\langle X A_i \right\rangle - \left\langle X \right\rangle \left\langle A_i \right\rangle$$

Derivatives: an example



PRD 92 (2015) 11, 114505 ; Bellwied, Borsanyi, Fodor, Katz, Pasztor, Ratti, Szabo

- 4th order in the continuum: 2015
- 6th order in the continuum: 2023
- 8th order: only at a finite lattice spacing so far
- Higher orders: worse signal-to-noise ratio
- Suppose we can calculate to high orders, what limits the convergence?

Canonical partition functions and Lee-Yang zeros

- For simplicity: only one charge N.
- Since $[H, N] = 0$ we can simultanously diagonalize
- The partition function:

$$\mathcal{Z} = \text{Tr}\left(e^{-(H-\mu N)/T}\right) = \sum_{n=-kV}^{+kV} e^{n\mu/T}\,\text{Tr}_n(e^{-H/T}) = \sum_n Z_n e^{n\mu/T}$$

- $\text{Tr}_n(\dots) =$ trace over state $|\psi\rangle \in \mathcal{H}$ s.t. $N|\psi\rangle = n\||\psi\rangle$
- Z is (up to a non-vanishing factor) a polynomial in $e^{\mu/T}$
- Polynomial $\rightarrow$ has $2kV$ roots in the complex fugacity plane $\rightarrow$ Lee-Yang zeros
- $Z \propto \prod_{i=1}^{2kV}(z_n - e^{\mu/T}) \propto \prod_{i=1}^{\infty}(w_i - \mu/T)$
- Z has $\mu \rightarrow -\mu$ symmetry (charge conjugation)
- $Z_n \in \mathbf{R} \rightarrow$ Lee-Yang zeros come in complex conjugate pairs
- At the LY zeros $\log Z$ has a branch point singularity, this gives the radius of convergence
- Finite volume scaling of LY zeros $\rightarrow$ order of transition

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Roberge-Weiss symmetry

- Put μ on the last time-slice for all quarks: $e^{i\mu_I/T}$
- Center transformation on final slice $z^k = e^{\frac{2\pi ik}{N}} \to e^{i\left(\frac{\mu_I}{T}+\frac{2\pi k}{M}\right)}$
- The determinant satisfies:

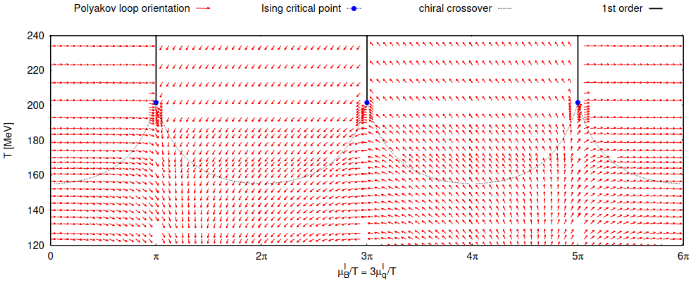
$$\det M(z^k U, \frac{\mu}{T}) = \det M(U, \frac{\mu}{T} + \frac{2\pi ik}{N})$$

- Thus:

$$\begin{aligned} Z\left(\frac{\mu}{T}\right) &= \int \mathcal{D}U \det M(U, \mu/T) e^{-S_G(U)} \\ &= \int \mathcal{D}(z^k U) \det M(z^k U, \mu/T) e^{-S_G(z^k U)} = \\ &= \int \mathcal{D}U \det M(U, \mu/T + i2\pi k/N) e^{-S_G(U)} = Z(\frac{\mu}{T} + \frac{2\pi ik}{N}) \end{aligned}$$

It is natural to write the free energy as a Fourier series.
Note: from just $Z = Tr(e^{-(H-\mu_q N_q)/T})$ one would naively expect $N = 3$ times the period (Spectrum has baryons, NOT quarks.)

Phase diagram at imaginary μ_B



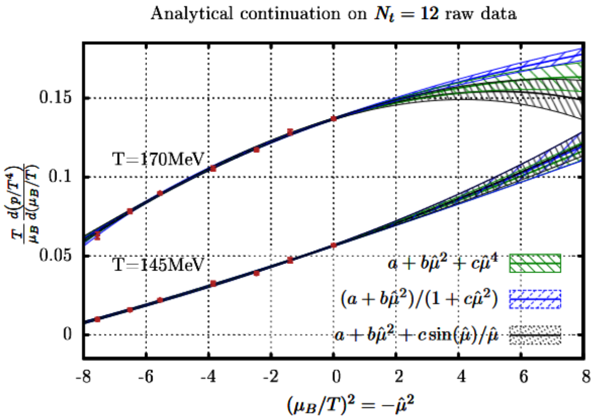
Matsubara frequencies:

$$(2n+1+0)\pi T + \mu_I \quad (2n+1+2/3)\pi T + \mu_I \quad (2n+1-2/3)\pi T + \mu_I$$

Magnitude of lowest frequency largest for:

$\phi_1 = 0$	$-\pi/3 < \mu_I/T < \pi/3$
$\phi_1 = -2\pi/3$	$\pi/3 < \mu_I/T < \pi$
$\phi_1 = 2\pi/3$	$-\pi < \mu_I/T < -\pi/3$

Imaginary μ as an extrapolation tool

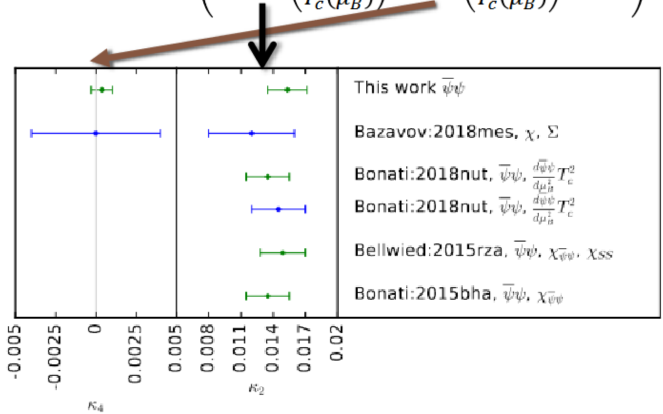


Two uses:

- Numerical differentiation at $\mu = 0$: safe
- Extrapolation: risky

The curvature of the crossover line

$$T_c(\mu_B) = T_c(0)\left(1 - \kappa_2\left(\frac{\mu_B}{T_c(\mu_B)}\right)^2 - \kappa_4\left(\frac{\mu_B}{T_c(\mu_B)}\right)^4 - \cdots\right)$$

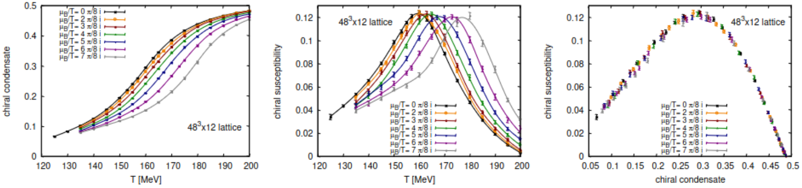


W-B: PRL 125 (2020) 5, 052001; 2002.02821

These are for μ_s tuned such that $\langle S \rangle = 0$.

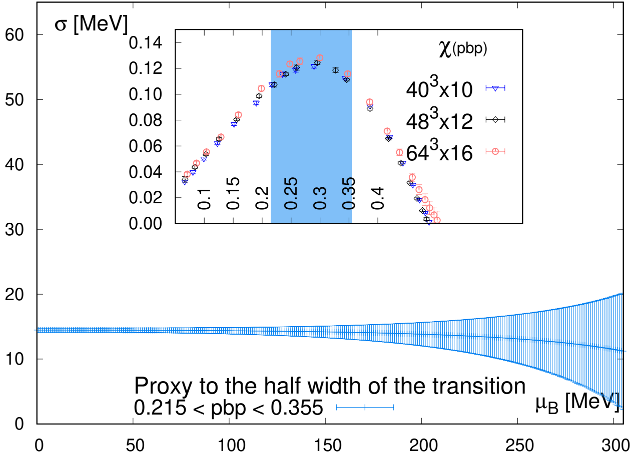
The CEP is not a special point of this curve, but it should lie on it.

The curvature of the crossover line - analysis sketch



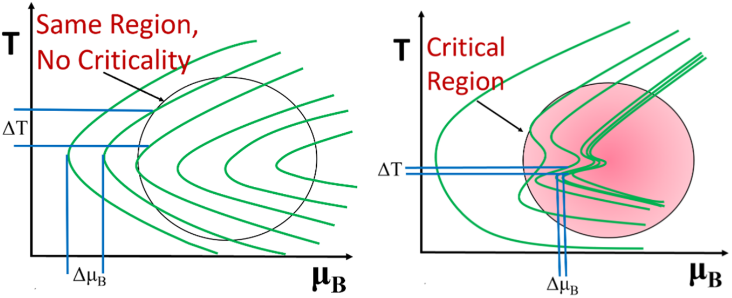
1) Tune μ_S for each T and μ_B such that $\chi_1^S = 0$
2) 2D scan in T and $\mathrm{Im}\,\mu_B \to \chi(\langle\bar\psi\psi\rangle)$
3) Peak of $\chi(\bar\psi\psi)$ through a low-order polynomial fit for each N_τ and $\mathrm{Im}\,\mu_B \to \langle\bar\psi\psi\rangle_c(N_t, \mathrm{Im}\,\mu_B)$
4) Interpolate $\langle\bar\psi\psi\rangle$ to convert $\langle\bar\psi\psi\rangle_c$ to T_c for each $\mathrm{Im}\,\mu_B/T$
5) Global fit of $T_c(Nt, \mathrm{Im}\,\mu_B/T_c)$ to determine κ_2 and κ_4 for $1/N_t^2 = 0$

The width of the crossover at small μ_B



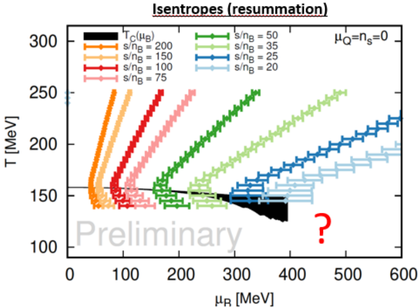
Wuppertal-Budapest: PRL 125 (2020) 5, 052001;

Isentropes: critical lensing



Sketch from Dore et al, PRD106 (2022)

Isentropes from analytic continuation



RHIC freeze-out [STAR, PRC96 (2017)]

$\sqrt{s} = 19.6\text{GeV} \leftrightarrow \mu_B \approx 200\text{MeV}$

$\sqrt{s} = 11.5\text{GeV} \leftrightarrow \mu_B \approx 300\text{MeV}$

$\sqrt{s} = 7.7\text{GeV} \leftrightarrow \mu_B \approx 400\text{MeV}$

No sign of critical lensing within errors

Wuppertal-Budapest (preliminary)

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Reweighting

Fields: ϕ Target theory: Z_t Simulated theory: Z_s

$$Z_t = \int \mathcal{D}\phi \; w_t(\phi) \qquad w_t(\phi) \in \mathbb{C}$$

$$Z_s = \int \mathcal{D}\phi \; w_s(\phi) \qquad w_s(\phi) > 0$$

$$\frac{Z_t}{Z_s} = \left\langle \frac{w_t}{w_s} \right\rangle_s$$

$$\langle O \rangle_t = \frac{\int \mathcal{D}\phi \; w_t(\phi) O(\phi)}{\int \mathcal{D}\phi \; w_t(\phi)} = \frac{\int \mathcal{D}\phi \; w_s(\phi) \frac{w_t(\phi)}{w_s(\phi)} O(\phi)}{\int \mathcal{D}\phi \; w_s(\phi) \frac{w_t(\phi)}{w_s(\phi)}} = \frac{\left\langle \frac{w_t}{w_s} O \right\rangle_s}{\left\langle \frac{w_t}{w_s} \right\rangle_s}$$

Two problems that are exponentially hard in the volume can arise:

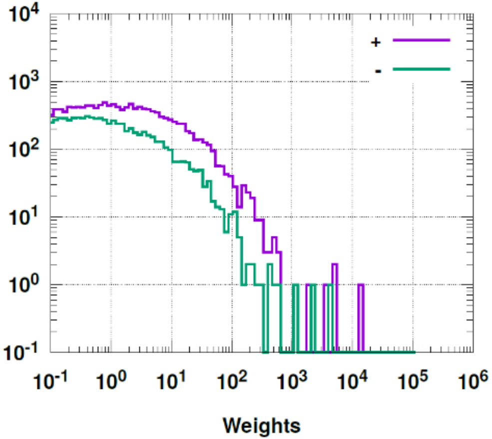
- $\frac{w_t}{w_s} \in \mathbb{C} \rightarrow$ the complex action problem became a **sign problem**
- Tails of $\rho(\frac{w_t}{w_s})$ long $\rightarrow$ **overlap problem**
- Important to choose a "good" w_s

The overlap problem

The expectation value of any observable:

$$\langle O \rangle_t = \frac{\left\langle \frac{w_t}{w_s} O \right\rangle_s}{\left\langle \frac{w_t}{w_s} \right\rangle_s}$$

The weights are the $\frac{w_t}{w_s} \propto \frac{\det M(\mu)}{\det M(0)}$. To calculate anything, we need to have control over this observable



Giordano, Kapas, Katz, Nogradi, Pasztor; PRD 102, 034503 (2020)

Phase and sign reweighting

A simple way to avoid long tails for the distribution of $\frac{w_t}{w_s}$ is to make sure that w_t/w_s take values from a compact space.

Phase reweighting

$$\begin{aligned} w_t &= e^{-S_g} \det M = e^{-S_g} |\det M| e^{i\theta} \\ w_s &= e^{-S_g} |\det M| \quad \text{phase quenched ensemble} \end{aligned} \quad \Rightarrow \quad \frac{w_t}{w_s} = e^{i\theta}$$

Severity of the sign problem: $\left\langle e^{i\theta} \right\rangle_{\rm PQ} = \langle \cos\theta \rangle_{\rm PQ}$
Hard to simulate

Sign reweighting

$$\begin{aligned} w_t &= e^{-S_g} \mathrm{Re} \det \mathrm{M} \\ w_s &= e^{-S_g} |\mathrm{Re} \det \mathrm{M}| \quad \text{sign quenched ensemble} \end{aligned} \quad \Rightarrow \quad \frac{w_t}{w_s} = \operatorname{sgn} \cos\theta = \pm 1$$

$\det M \to \mathrm{Re} \det M$ can be done in Z but not in generic expectation values. E.g. things like $\frac{\partial^n \log Z}{\partial \mu_{ud}^n}$, $\frac{\partial^n \log Z}{\partial m_{ud}^n}$ and $\frac{\partial^n \log Z}{\partial \beta^n}$ can be calculated.

Severity of the sign problem: $\langle \pm \rangle_{\rm SQ}$
de Forcrand et al; NPB Proc. S. 119, 541 (2003) - optimal choice for $\frac{w_t}{w_s} = f(\theta)$

BUT: hard to simulate with weights $\propto |\mathrm{Re} \det \mathrm{M}|$

The sign problem

- From PQ: $\frac{Z}{Z_{PQ}} = \left\langle e^{i\theta} \right\rangle$
- Locality $\rightarrow$ central limit theorem (on the circle, the only stable distribution is the uniform)
- For fermionic theories, the observables can also be problematic:

$$\frac{\partial^n}{\partial \mu^n} \log Z \ni \left\langle \frac{\partial}{\partial \mu^n} \log \det M \right\rangle$$

  configs with $\det M \approx 0 \rightarrow$ bad signal-to-noise ratio
- Example: the determinant is real for non-zero isospin, but:
    - isospin density at non-zero isospin ✓
    - isospin susceptibility at non-zero isospin ✗
- Solution: polynomial time algorithm
- Troyer & Weise PRL94 (2005): generic sign problem is NP-hard
- BUT: generic is an important word here:
    - Specific sign problems can be solved, and have been solved
    - Generic looking ideas might solve it for some cases, but not others

The phase diagram for non-zero isospin

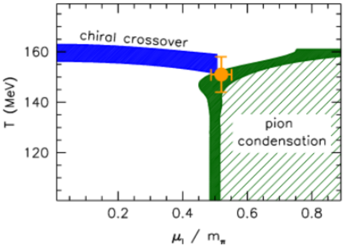
- $SU(2)_V$ broken by the isospin chemical potential to a $U(1)$:

$$D + m + \mu_I \gamma_0 \tau_3$$

- This is then spontaneously broken at a second order transition

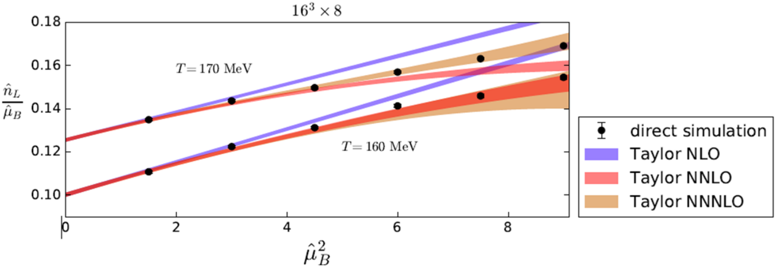
$$SU(2)_V \to U(1)_{\tau_3} \to \emptyset$$

- $\to$ 1 Goldstone mode
- Add explicit breaking $i\lambda\gamma_5\tau_2$
- Extrapolate $\lambda \to 0$ (similar to a χ lim)
- Sign problem most severe in the π condensed phase:
$\left\langle e^{i\theta} \right\rangle_{\mathrm{PQ}} = \frac{Z_{\mu_B}}{Z_{\mathrm{I}}} = e^{-V(f_{\mathrm{B}} - f_{\mathrm{I}})}$



Brandt, Endrődi, Schmalzbauer; PRD97, 054514 (2018)

Extrapolation vs direct results



Wuppertal-Budapest: Phys.Rev.D 107 (2023) 9, L091503

Conclusion: in the RHIC BES range (in collider mode) the QGP EoS is under control

Summary: $\mu_B > 0$

What is known

- 2nd and 4th derivatives in continuum, 6th and 8th order at finite a
- curvature of the crossover line
- the strength of the crossover $\approx$ const. at small μ
- EoS in the experimentally accessible range (RHIC BES)

Ongoing research: analytic continuation methods

- Higher order Taylor coefficients at $\mu = 0$
- Higher order Fourier coefficients at imaginary μ
- Calculating Lee-Yang zeros and radius of convergence
- Resummations of the series beyond the

Ongoing research: direct methods

- A good discretization for $\mu > 0$?
- Approaches to the sign problem