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The QCD Phase Diagram

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Lecture I: QCD at finite temperature and density, continuum and lattice

Lecture II:Towards the QCD phase diagram at finite temperature and density

Literature

O.P., "Lattice QCD at non-zero temperature and density", Les Houches lecture notes 2009, arxiv:1009.4089

O.P., "The QCD equation of state from the lattice" Prog. Part. Nucl. Phys. 70 (2013) 55, arxiv:1207.5999

Proper references to covered material in those articles

Textbooks:

Gale, Kapusta, "Finite temperature field theory: principles and applications"

Montvay, Münster, "Quantum fields on a lattice"

Gattringer, Lang, "Quantum chromodynamics on the lattice"

Lecture I: QCD at finite temperature and density

Motivation: Why thermal QCD?

The continuum formulation

The lattice formulation

Phase transitions and phase diagrams

Why thermal QCD?



Thermal QCD in nature



What are compact stars made of?



Radius ~ 10-12 km Mass ~ 1.2-2.2 x Solar Mass



 ρ_0 : nuclear density

Thermal QCD in experiment



heavy ion collision experiments at RHIC, LHC, GSI....

QCD phase diagram: theorist's view (science fiction)



Until 2001: no finite density lattice calculations, sign problem!

Expectation based on simplifying models (NJL, linear sigma model, random matrix models, ...)

Check this from first principles QCD!

Less conservative views....



+ inhomogeneous phases, quarkyonic phases,.... you name it!

The QCD phase diagram established by experiment:



Nuclear liquid gas transition with critical end point

Unsolved from QCD: nuclear matter

~100 years old, still no fundamental description, Bethe-Weizsäcker droplet model:



QFT descriptions: Fetter-Walecka model, Skyrme model, ...

Statistical mechanics reminder

System of particles in volume V with conserved number operators, N_i , i = 1, 2, ... in thermal contact with heatbath at temperature T

Canonical ensemble: exchange of energy with bath, particle number fixed

Grand canonical ensemble: exchange of energy and particles with the bath

Density matrix,
Partition function:
$$\rho = e^{-\frac{1}{T}(H-\mu_i N_i)}$$
, $Z = \hat{T}r\rho$, $\hat{T}r(\ldots) = \sum_n \langle n|(\ldots)|n \rangle$ Thermodynamics: $F = -T \ln Z$,
 $p = \frac{\partial (T \ln Z)}{\partial V}$,
 $S = \frac{\partial (T \ln Z)}{\partial V}$,
 $S = \frac{\partial (T \ln Z)}{\partial T}$, $\bar{N}_i = \frac{\partial (T \ln Z)}{\partial \mu_i}$,
 $E = -pV + TS + \mu_i \bar{N}_i$ Densities: $f = \frac{F}{V}$, $p = -f$, $s = \frac{S}{V}$, $n_i = \frac{\bar{N}_i}{V}$, $\epsilon = \frac{E}{V}$

QCD at finite temperature and density

Grand canonical partition function

$$Z(V,T,\mu;g,N_f,m_f) = \operatorname{Tr}(\mathrm{e}^{-(\mathrm{H}-\mu\mathrm{Q})/\mathrm{T}}) = \int \mathrm{DA}\,\mathrm{D}\bar{\psi}\,\mathrm{D}\psi\,\mathrm{e}^{-\mathrm{S}_{\mathrm{g}}[\mathrm{A}_{\mu}]}\mathrm{e}^{-\mathrm{S}_{\mathrm{f}}[\bar{\psi},\psi,\mathrm{A}_{\mu}]}$$

Action

$$S_{g}[A_{\mu}] = \int_{0}^{1/T} d\tau \int_{V} d^{3}x \, \frac{1}{2} \text{Tr} \, F_{\mu\nu}(x) F_{\mu\nu}(x),$$
$$S_{f}[\bar{\psi}, \psi, A_{\mu}] = \int_{0}^{1/T} d\tau \int_{V} d^{3}x \, \sum_{f=1}^{N_{f}} \bar{\psi}_{f}(x) \left(\gamma_{\mu} D_{\mu} + m_{f} - \mu_{f} \gamma_{0}\right) \psi_{f}(x)$$

$$A_{\mu}(\tau, \mathbf{x}) = A_{\mu}(\tau + \frac{1}{T}, \mathbf{x}), \qquad \psi_f(\tau, \mathbf{x}) = -\psi_f(\tau + \frac{1}{T}, \mathbf{x}) \qquad \text{quark number} \qquad N_q^f = \bar{\psi}_f \gamma_0 \psi_f$$

Parameters

$$g^2, m_u \sim 3 \text{MeV}, m_d \sim 6 \text{MeV}, m_s \sim 120 \text{MeV}, V, T, \mu = \mu_B/3$$

 $N_f = 2 + 1$ sufficient up to T~300-400 MeV

Symmetries of the QCD Lagrangian



Global axial U(1) transformations, anomalous, broken by quantum effects

Symmetries for parameter values realised by nature

 $SU(3)_c$ gauge symmetry, exact, only colour singlets observable $U(1)_{B}$ baryon number, exact $SU(2)_{\rm isospin}$ approximate, O(few %), $m_u \approx m_d$ $SU(3)_{\text{flavour}}$ $m_u \approx m_d \sim m_s$ (quark model!) approximate, O(few 10 %), $m_u \approx m_d \approx 0$ $SU(2)_{\text{axial}}$ approximate approximate chiral symmetry $m_u pprox m_d pprox 0$ $SU(2)_L \times SU(2)_R$ = isospin+axial flavour symmetry combined

Perturbation theory at finite T

Split action into free (Gaussian) and interacting part, expand in interactions

$$Z = N \int D\phi \, e^{-(S_0 + S_i)} = N \int D\phi \, e^{-S_0} \sum_{l=0}^{\infty} \frac{(-1)^l}{l!} S_i^l$$

$$\ln Z = \ln Z_0 + \ln Z_i = \ln \left(N \int D\phi \, \mathrm{e}^{-S_0} \right) + \ln \left(1 + \sum_{l=1}^{\infty} \frac{(-1)^l}{l!} \frac{\int D\phi \, \mathrm{e}^{-S_0} S_i^l}{\int D\phi \, \mathrm{e}^{-S_0}} \right)$$

Renormalisation: Whatever renormalisation is necessary and sufficient at T=0 is also necessary and sufficient at finite temperature and density

UV behaviour: microscopic physics, depends on details of interactions

 T, μ : macroscopic parameters, affect IR behaviour of the theory

Difference to T=0: compact, periodic time direction!

Fourier expansion of the fields: discrete Matsubara frequencies

$$A_{\mu}(\tau, \mathbf{x}) = \frac{1}{\sqrt{VT}} \sum_{n=-\infty}^{\infty} \sum_{\mathbf{p}} e^{i(\omega_n \tau + \mathbf{p} \cdot \mathbf{x})} A_{\mu,n}(p) , \quad \omega_n = 2n\pi T , \qquad p_i = (2\pi n_i)/L$$
$$\psi(\tau, \mathbf{x}) = \frac{1}{\sqrt{V}} \sum_{n=-\infty}^{\infty} \sum_{\mathbf{p}} e^{i(\omega_n \tau + \mathbf{p} \cdot \mathbf{x})} \psi_n(p) , \quad \omega_n = (2n+1)\pi T$$

Thermodynamic limit:

$$\frac{1}{V} \sum_{n_1, n_2, n_3} \stackrel{V \to \infty}{\longrightarrow} \int \frac{d^3 p}{(2\pi)^3}$$

Modified Feynman rules:

Inverse (bosonic) free propagator:

$$\Delta^{-1} = p^2 + m^2 = \omega_n^2 + \mathbf{p}^2 + m^2 = (2n\pi T)^2 + \mathbf{p}^2 + m^2$$

Loop integration:



IR-structure: divergences and mass scales

Inverse (bosonic) free propagator:

Corrections:

$$p^2 + m^2 = \omega_n^2 + \mathbf{p}^2 + m^2 = (2n\pi T)^2 + \mathbf{p}^2 + m^2$$

f
effective thermal mass ~T

n=0 mode: propagator of a 3d theory, divergent for m=0!

 $m_E^{LO} = \left(\frac{N}{3} + \frac{N_f}{6}\right)^{1/2} gT$ electric or Debye screening mass $\langle A_0(\mathbf{x})A_0(\mathbf{y}) \rangle$ mass $m_M^{LO} = 0, m_M \sim g^2 T \quad \text{from 2-loop}$ magnetic screening mass $\langle A_i(\mathbf{x})A_i(\mathbf{y}) \rangle$

0-mode sector of 4d QCD at finite T contains 3d Yang-Mills theory with $g_3^2 \sim g^2 T$ Confining! Doom for perturbation theory....

Salvation comes as a lattice...



Lattice formulation of Euclidean QFT's

 $\mathbb{R}^4 \rightarrow x = \{x_\mu | \mu = 1, \dots, 4\} \in a\mathbb{Z}^4 \quad a : \text{ lattice spacing (or constant)}$



- $\phi(x)$: living on the lattice sites only
- partial derivatives \rightarrow finite differences:

$$\partial_{\mu}\phi \longrightarrow \Delta_{\mu}^{(*)}\phi(x) = \frac{\pm\phi(x\pm a\hat{\mu})\mp\phi(x)}{a}$$

 \Rightarrow forward & backward lattice derivatives

Rotation symmetry:
$$\int d^4 x \rightarrow \sum_x a^4 \qquad \mathcal{D}\phi \rightarrow \prod_x d\phi(x) \equiv \mathcal{D}[\phi]$$

 $SO(4) \longrightarrow D_h^4$

(infinite-dimensional) integration measure well defined on discrete system!



finite numbers on finite lattice!

SU(N) gauge theory on a lattice



Gauge trafo: $\psi^g(x) = g(x)\psi(x)$, $U^g_\mu(x) = g(x)U_\mu(x)g^{\dagger}(x+\hat{\mu})$

Covariant derivative:

$$D_{\mu}\psi(x) \to a^{-1} \left(U_{\mu}(x)\psi(x+\hat{\mu}) - \psi(x) \right) + O(a)$$



smallest loop: "plaquette" $U_p(x) \equiv U^{\dagger}(x, \mathbf{v})U^{\dagger}(x + a\hat{\mathbf{v}}, \mu)U(x + a\hat{\mu}, \mathbf{v})U(x, \mu)$

$$\Box \to 1 + ia^2 g F_{\mu\nu} - \frac{a^4 g^2}{2} F_{\mu\nu} F^{\mu\nu} + O(a^6) + \dots$$
$$U_{\mu}(x) = e^{-iagA_{\mu}(x)}$$

$$\Box \to 1 + ia^2 g F_{\mu\nu} - \frac{a^4 g^2}{2} F_{\mu\nu} F^{\mu\nu} + O(a^6) + \dots$$

Wilson action:

$$S_{g}[U] = \beta \sum_{p} \left\{ 1 - \frac{1}{N} \operatorname{Re} \left[\operatorname{Tr} U(p) \right] \right\} \qquad \sum_{p} = \sum_{x} \sum_{1 \le \mu < \nu \le 4}$$
$$\beta = \frac{2N}{g^{2}} \qquad \text{lattice gauge coupling}$$

reproduces SU(N) Yang-Mills in continuum limit; for finite a not unique!

- action gauge-invariant for any lattice spacing
- real, positive

Adding fermions



Wilson fermions:

$$S_f^W = \frac{1}{2a} \sum_{x,\mu,f} a^4 \,\bar{\psi}_f(x) [(\gamma_\mu - r) U_\mu(x) \psi_f(x + \hat{\mu}) - (\gamma_\mu + r) U_\mu^\dagger(x - \hat{\mu}) \psi_f(x - \hat{\mu})]$$

$$+\left(m+4\frac{r}{a}\right)\sum_{x,f}a^{4}\,\bar{\psi}_{f}(x)\psi_{f}(x)$$

pick your poison

Wilson fermions

add irrelevant ops. (going away in CL) to make doublers very massive breaks chiral symmetry for non-zero a

staggered (Kogut-Susskind) fermions

distribute spinor components on different sites, reduces to 4 flavours take 4th root of determinant to get to one flavour, keeps reduced chiral symm. non-local operation, have to take CL before chiral limit, mixing of spin, flavour

domain wall fermions

introduce 5th dimension, fermions massive in that dim. and chiral in the other expensive

overlap fermions non-local formulation with modified chiral symmetry even for finite a order of magnitude more expensive than Wilson

Monte Carlo evaluation

Euclidean partition function:

$$Z = \int D\bar{\psi}D\psi DU \,\mathrm{e}^{-S_g[U] - S_f[U,\bar{\psi},\psi]} = \int DU \,\prod_f (\det M) \,\mathrm{e}^{-S_g[U]}$$

Systematics: finite V,a effects

for hadron with m_H , $\xi \sim m_H^{-1}$ $a \ll \xi \ll aL$!



 \Rightarrow e.g. $30^4 \sim 10^6$ lattice points

every point \Rightarrow 4 U's, every $U \in$ SU(3) \Rightarrow 8 independent components \Rightarrow 10⁸-dimensional integral!

Directly calculable: particle masses, decay constants, equilibrium thermodynamics

 \Rightarrow Monte Carlo integration, importance sampling

Markov process: ensemble $\{U_1\} \rightarrow \{U_2\} \rightarrow \{U_3\} \dots \{U_N\}$

" \rightarrow ": updating algorithm with associated probability, ergodic

$$\det M[U]e^{-S[U]}$$

U

$$\langle \mathcal{O} \rangle = Z^{-1} \int DU \det M \mathcal{O} e^{-S_g[U]} \approx \frac{1}{N} \sum_{n=1}^{N} (\det M \mathcal{O})[U]$$

 $\Rightarrow N$ "measurements" of \mathcal{O} \Rightarrow statistical error $\sim 1/\sqrt{N}$

Light fermions expensive:

$$\det M[U] = \lambda_1[U] \cdot \lambda_2[U] \cdot \lambda_3[U] \dots, \quad \operatorname{cost}(\det M) \sim \frac{1}{m_q^n}, \quad n > 5$$

Non-local: every eigenvalue depends on every link

Continuum limit

$$\frac{1}{T} \equiv aN_{\tau}$$

Fixed scale approach:

For a given lattice spacing, N_{τ} controls temperature;

Allows only discrete temperatures, too large for many applications;

Continuum limit requires series of lattice spacings

Fixed N_{τ} approach:

For a given $N_{ au}$, vary the lattice spacing via eta(a);

Allows continuous temperatures, but each T value has different cut-off!

Continuum limit requires series of $N_{ au}$

Quenched limit of QCD and Z(N) symmetry

Infinite quark masses (omitting flavour index) $m \to \infty$

Static quark propagator:
$$\langle \psi^a_{\alpha}(\tau, \mathbf{x}) \bar{\psi}^b_{\beta}(0, \mathbf{x}) \rangle = \delta_{\alpha\beta} e^{-m\tau} \left(T e^{i \int_0^{\tau} d\tau A_0(\tau, \mathbf{x})} \right)_{ab}$$

On the finite T lattice:

Polyakov loop $L(\mathbf{x}) = \prod U_0(x)$

$$\begin{split} S_{\text{static}}[U] &= S_g[U] + \sum_{\mathbf{x}} \left(e^{-mN_{\tau}} \operatorname{Tr} L(\mathbf{x}) + e^{-mN_{\tau}} \operatorname{Tr} L^{\dagger}(\mathbf{x}) \right) \\ \stackrel{m \to \infty}{\longrightarrow} S_g[U] \end{split}$$

 N_{τ}

 x_0

Gauge transformations:

Periodic b.c.:

$$U^{g}_{\mu}(x) = g(x)U_{\mu}(x)g^{-1}(x+\hat{\mu}), \quad g(x) \in SU(N)$$
$$U_{\mu}(\tau, \mathbf{x}) = U_{\mu}(\tau + N_{\tau}, \mathbf{x}), \quad g(\tau, \mathbf{x}) = g(\tau + N_{\tau}, \mathbf{x})$$

Action gauge invariant:

 $S_g[U^g] = S_g[U] \qquad L^g(\mathbf{x}) = g(x)L(\mathbf{x})g^{-1}(x) \qquad \mathrm{Tr}L^g = \mathrm{Tr}L$

Topologically non-trivial gauge transformations:

Modified b.c. for trafo matrix:
$$g'(au+N_{ au},\mathbf{x})=hg'(au,\mathbf{x})\,,\quad h\in SU(N)$$

$$\uparrow$$
global "twist"

 $U^{g'}_{\mu}(\tau + N_{\tau}, \mathbf{x}) = h U^{g'}_{\mu}(N_{\tau}, \mathbf{x}) h^{-1}$ needs to be periodic for correct finite T physics!

$$h = z1 \in Z(N), \quad z = \exp i \frac{2\pi n}{N}, \quad n \in \{0, 1, 2, \dots N - 1\}$$
 Centre of SU(N)

 $S_g[U^{g'}] = S_g[U]$ invariant: centre symmetry of pure gauge action

Note: this is not a symmetry of H

Requires compact time direction with periodic b.c.; finite T!

$$L^{g'}(\mathbf{x}) = g'(1, \mathbf{x})L(\mathbf{x})g'^{-1}(1 + N_{\tau}, \mathbf{x}) = g'(1, \mathbf{x})L(\mathbf{x})g'^{-1}(1, \mathbf{x})h^{-1}$$

 $\text{Tr}L^{g'} = z^* \text{Tr}L$ Polyakov loop picks up a phase under centre transformations

Partition function in the presence of one static quark: $Z_Q = \int DU \operatorname{Tr} L(\mathbf{x}) e^{-S_g[U]}$

$$\langle \mathrm{Tr}L \rangle = \frac{1}{Z} \int DU \,\mathrm{Tr}L \,\mathrm{e}^{-S_g} = \frac{Z_Q}{Z} = \mathrm{e}^{-(F_Q - F_0)/T}$$

gives free energy difference of thermal YM-system with and without a static quark



Deconfinement phase transition in YM: spontaneous breaking of Z(N) symmetry

Now add dynamical quarks:

$$\psi^{g}(x) = g(x)\psi(x), \quad \psi(\tau + N_{\tau}, \mathbf{x}) = -\psi(\tau, \mathbf{x}), \quad \psi^{g'}(\tau + N_{\tau}, \mathbf{x}) = -h\psi(\tau, \mathbf{x})$$

needs to be anti-periodic for correct finite T physics! h = 1 only



Centre symmetry explicitly broken by dynamical quarks!

$$\langle \text{Tr}L \rangle \neq 0$$
 for all T!



Confined and deconfined region analytically connected (only one phase!) No need for a phase transition!

Physical QCD

.....breaks both chiral and Z(3) symmetry explicitly

.....but displays confinement and very light pions

no order parameter no phase transition necessary!

if there is a p.t.: are there two distinct transitions?

- if there is just one p.t.: is it related to chiral or Z(3) dynamics?
- if there is no phase transition: how do the properties of matter change?

Phase transitions and phase diagrams

- phase transitions: singularities in free energy $F \Rightarrow$ zeroes in partition function Z only in thermodynamic limit! (Lee, Yang)
- first order: jump in order parameter, latent heat, phase coexistence
- second order: diverging correlation length
- crossover smooth, analytic transition

Example 1: water



Example 2: ferromagnetism



Ising model, Z(2) symmetry

spins with nearest neighbour interaction

$$E = -\sum_{ij} \epsilon_{i,j} s_i s_j - H \sum_i s_i$$

$$t = (T - T_c)/T_c$$

Universality of 2.o. phase transitions, critical exponents:

Correlation length diverges: microscopic dynamics unimportant, only global symmetries specific heat $C \sim |t|^{-\alpha}$, magnetization $M \sim |t|^{\beta}$, $\chi \sim |t|^{-\gamma}$ and $\xi \sim |t|^{-\nu}$ exponents the same for all systems within one universality class! Critical endpoint of water shows 3d Ising universality, Z(2)!

Scaling analyses employing universality

Effective Hamiltonian analogous to Ising model:

$$\frac{H_{eff}}{T} = \tau E + hM$$

Extensive operators:E energy-likeM magnetisation-likeParameters: τ temperature-likeh magnetic field-like

At a critical point, the singular part of the free energy has the scaling form:

 $f_s(\tau, h) = b^{-d} f_s(b^{D_\tau} \tau, b^{D_h} h)$ $b = LT = N_s/N_\tau$ dim.less scale factor

Relation between scaling dimensions and critical exponents:

$$D_{\tau} = \frac{1}{\nu}, \quad \gamma = \frac{2D_h - d}{D_{\tau}}, \quad \alpha = 2 - \frac{d}{D_{\tau}}$$



$$\chi_E = V^{-1} \langle (\delta E)^2 \rangle = -\frac{1}{T} \frac{\partial^2 f}{\partial \tau^2} \sim b^{\alpha/\nu},$$
$$\chi_M = V^{-1} \langle (\delta M)^2 \rangle = -\frac{1}{T} \frac{\partial^2 f}{\partial h^2} \sim b^{\gamma/\nu}$$

How to map parameters and fields of QCD to those of the Ising model?

For many applications not necessary...

 $E(S_p, \overline{\psi}\psi, \ldots), M(S_p, \overline{\psi}\psi, \ldots), \tau(\beta, m_f, \mu_f), h(\beta, m_f, \mu_f))$



 $\chi_{ar{\psi}\psi}(E,M)$ mix of energy and magnetic susceptibilities, in thermodynamic limit the more divergent one dominates!

Symmetry groups relevant for QCD: Z(2), O(4), O(2)



 $\chi_{\bar{O}} \sim V$ First order scaling:

Analytic crossover:

no divergence, susceptibilities have finite thermodynamic limit

Finding a phase transition in QCD: fluctuations



Monte Carlo history, plaquette near phase boundary



first-order



crossover





Summary Lecture I

- QCD at finite temperature and density important for many fields of physics
- Perturbation theory for finite T QFT limited, infrared modes always confining!
- Solution by Monte Carlo simulation of lattice QCD at finite T
- Phase transitions: finite size scaling analyses