# Lattice QCD at non-zero temperature and density

Frithjof Karsch

Bielefeld University & Brookhaven National Laboratory

- QCD in a nutshell, non-perturbative physics, lattice-regularized QCD, Monte Carlo simulations
- the phase diagram on strongly interacting matter, chiral symmetry restoration, the equation of state
- finite density QCD, cumulants of conserved charge fluctuations, thermal masses & transport properties

## Literature

- M. Creutz, Quarks, Gluons and Lattices
- H. Rothe, Lattice Gauge Theories
- T. DeGrand, C. DeTar, Lattice Methods for Quantumchromodynamics
- C. Gattringer and C.B. Lang, Quantum Chromodynamics on the Lattice
- I. Montvay, G. Muenster, Quantum Fields on a Lattice
- J. Zinn-Justin, Quantum Field Theory and Critical Phenomena
- H.T. Ding, FK, S. Mukherjee, Thermodynamics of strong-interaction Matter from Lattice QCD, Int. J. Mod. Phys. E24 (2015) 153007

# Motivation

## Why lattice (gauge) theory?

Many phenomena in physics are of 'non-perturbative' nature

- Spontaneous symmetry breaking:
  - Phase transitions (spontaneous magnetization, Ising model)
  - Higgs mechanism
  - chiral symmetry breaking
- The origin of mass, hadron spectra
  - $m_{u,d} \simeq 5$  MeV, but  $m_p = 938\,$  MeV
- Long distance properties of Quantum Field Theories
  - confinement, screening

# The theory of strong-interaction Quantum Chromo Dynamics (QCD)

 $\mathcal{J} = \frac{1}{4g^2} G_{\mu\nu} G_{\mu\nu} + \sum_j \overline{g}_j (i \partial^{\mu} D_{\mu} + m_j) q_j$ where  $G_{\mu\nu}^{\alpha} \equiv \partial_{\mu} P_{\nu}^{\alpha} - \partial_{\nu} P_{\mu}^{\alpha} + i \int_{\partial \alpha}^{\alpha} P_{\mu}^{b} P_{\nu}^{c}$ and  $D_{\mu} \equiv \partial_{\mu} + i t^{\alpha} P_{\mu}^{\alpha}$ That's it!

F. Wilczek, QCD made simple, Phys. Today 53N8 (2000) 22

# The theory of strong-interaction Quantum Chromo Dynamics (QCD)

- non-abelian gauge theory, constructed in analogy to QED
- matter fields (quarks [fermions]) and force carrier (gluons [bosons])
- a new quantum number color  $N_c = r, b, g$
- quarks live in the fundamental representation of the SU(3) color group:
  - each quark species/flavor carries one of three possible colors
- gluons live in the adjoint representation; there are 8 different gluons
  - unlike the photon in QED the gluons not only interact with quarks but also among themselves
    - (three- and four-gluon vertices)

#### **Standard Model of Elementary Particles**





# The theory of strong-interaction Quantum Chromo Dynamics (QCD) – confinement --



Y. Aoki et al, Nature 443 (2006) 675

Hadrons in a thermal heat bath



H.-T. Ding et al., Phys. Rev. D86 (2012) 014509





thermodynamics of a hadron resonance gas

physics of the early universe



thermodynamics of a hadron resonance gas



## **Quantum Chromo** Dynamics (QCD)

– QCD is expected to explain ALL aspects of strong interaction physics

- a rich spectrum of hadrons (including the values of their masses)

- the peculiar role of the lightest hadrons  $\rightarrow$  pions
- the mass splitting among parity partners
- the mass-splitting of pion and delta (a\_0)

spontaneous breaking of chiral symmetries

 the absence of its basic constituents (quarks and gluons) from the experimentally observed particle spectrum

confinement

- the simple properties of deep inelastic scattering

asymptotic freedom

- the existence (?) of phase transitions

deconfinement & chiral symmetry resoration

## Lattice regularized **Quantum Chromo** Dynamics (**QCD**)

- start with the Euclidean version of the QCD Lagrangian:

$$Z(g^{2}, \{m_{f}\}_{f=1}^{n_{f}}) = \int \mathcal{D}\mathcal{A}\mathcal{D}\psi \mathcal{D}\bar{\psi} e^{-S_{E}}, S_{E} \equiv \int d^{4}x \mathcal{L}_{E}(x)$$

$$\gamma^{k} \rightarrow i\gamma_{k}^{E}, \ k-1, 2, 3 \qquad t = |t|e^{-i\theta}$$

$$dt \rightarrow d|t|e^{-i\theta}$$

$$dt \rightarrow d|t|e^{-i\theta}$$

$$\frac{d}{dt} \rightarrow \frac{d}{d|t|}e^{i\theta}$$
Ret

$$\mathcal{L}_E = rac{1}{4} F^a_{\mu
u} F^a_{\mu
u} + ar{\psi}_{j,a} \left( \sum_{
u=0}^3 \gamma_
u \left( \partial_
u - i rac{g}{2} \mathcal{A}^a_
u \lambda^a 
ight) + m_j 
ight)^{a,b} \psi_{j,b}$$

field strength tensor:  $F^a_{\mu\nu} = \partial_\mu \mathcal{A}^a_
u - \partial^a_
u \mathcal{A}^a_\mu - g f_{abc} \mathcal{A}^b_\mu \mathcal{A}^c_
u$ 

gluons: real 4-vector  $\mathcal{A}^a = (\mathcal{A}^a_0, ..., \mathcal{A}^a_3)$  a = 1, ..., 8quarks: 4-spinor, Grassmann variables  $\psi_{f,a}$ , a = 1, 2, 3, f = u, d, c, s, t, b

#### **Gauge** field theories

gauge transformation:  $G(x)\equiv {
m e}^{i\Lambda(x)}\in SU(3)~,~~\Lambda=\sum_{lpha=1}^{N_c^2-1}\Lambda^lpharac{\lambda^lpha}{2}$ 

complex  $N_c imes N_c$  matrix: G

 $G^{-1} = G^{\dagger}$  ,  $\det G = 1$ 

$$\begin{split} \psi(x) &\to G(x)\psi(x) \\ \bar{\psi}(x) &\to \bar{\psi}(x)G^{-1}(x) \Rightarrow \bar{\psi}(x)\psi(x) \text{ is gauge invariant} \\ A_{\mu}(x) &\to G(x)A_{\mu}(x)G^{-1}(x) - \frac{i}{g}G(x)\partial_{\mu}G^{-1}(x) \\ D_{\mu}(x) &\to G(x)D_{\mu}(x)G^{-1}(x) \Rightarrow \bar{\psi}(x)D_{\mu}(x)\psi(x) \text{ is gauge invariant} \end{split}$$

$$\Rightarrow~F'_{\mu
u}=GF_{\mu
u}G^{-1}\Rightarrow~{
m Tr}F_{\mu
u}F_{\mu
u}$$
 is gauge invariant

## The idea of K. Wilson: lattice gauge theory

regularize QCD by introducing a discrete space-time lattice;

- violates various symmetries, but...
- minimal requirement: preserve "local" gauge invariance

Phys. Rev. D 10 (1974) 2445

#### parallel transporter:

introduce gauge fields that interpolate between sites n and  $n + \mu$  $U(n, n + \mu) \equiv U_{n,\mu} \equiv U_{\mu}(n) = e^{ig \int_x^{x+\mu} dz A_{\mu}(z)} = e^{igaA_{\mu}(n)}$ 

gauge transformation:  $U_{\mu}(n) \rightarrow G_n U_{\mu}(n) G_{n+\mu}^{-1}$ 

I) introduce gauge degrees of freedom (vector fields) on links

$$egin{array}{c} U_\mu(n) \ h & n & n+\mu \end{array} \hspace{0.5cm} U_\mu(n) = \mathrm{e}^{i heta_\mu(n)} \hspace{0.5cm}, \hspace{0.5cm} heta_\mu(n) = gaA_\mu(n)$$

ii) replace gauge fields  $A_{\mu}(n) \equiv A^a_{\mu}(n) \lambda^a/2$  by elements of the relevant symmetry group

QCD: 
$$U_{n,\mu} \in SU(3)$$



lattice

spacing

#### lattice discretization:

introduce gauge degrees of freedom on links,

$$U_{\mu}(n) \in SU(N_c) \; , \; U_{\mu}(n) \equiv \mathrm{e}^{iagA_{\mu}(n)}$$
  
 $N_c imes N_c$  matrix



the plaquette variable Re Tr  $U_{\mu\nu}(n)$ 

#### lattice discretization:

introduce gauge degrees of freedom on links



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use Baker-Hausdorff repeatedly

$$\Rightarrow \text{ Re Tr} U_{\mu\nu}(n) = N_c - a^4 \frac{g^2}{2} \text{ Tr } F_{\mu\nu}(n) F_{\mu\nu}(n) + \mathcal{O}(a^6)$$

$$S_G = \frac{2N_c}{g^2} \sum_n \sum_{1 \le \mu < \nu \le 4} \left( 1 - \frac{1}{N_c} \operatorname{Re} \operatorname{Tr} U_{\mu\nu}(n) \right) \to \int \mathrm{d}^4 x \mathcal{L}_G(x) + \mathcal{O}(a^2)$$

$$Z(\beta) = \int \prod_{n,\mu} dU_{\mu}(n) e^{-S_G(U)} , \ \beta \equiv \frac{2N_c}{g^2} \qquad \begin{bmatrix} \text{not the} \\ \text{inverse} \\ \text{temperature!!} \end{bmatrix}$$

$$U_{\mu\nu}(n) \equiv U_{\mu}(n)U_{\nu}(n+\mu)U_{\mu}^{\dagger}(n+\mu)U_{\nu}^{\dagger}(n)$$

$$= e^{iagA_{\mu}(n)}e^{iagA_{\nu}(n+\mu)}e^{-iagA_{\mu}(n+\mu)}e^{-iagA_{\nu}(n)}$$

$$= e^{iag(A_{\mu}(n)+A_{\nu}(n+\mu))-a^{2}g^{2}[A_{\mu}(n),A_{\nu}(n+\mu)]}$$

use Baker-Hausdorff repeatedly

$$\Rightarrow \text{ Re Tr} U_{\mu\nu}(n) = N_c - a^4 \frac{g^2}{2} \text{ Tr } F_{\mu\nu}(n) F_{\mu\nu}(n) + \mathcal{O}(a^6)$$

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$$Z(eta) = \int \prod_{n,\mu} dU_{\mu}(n) \mathrm{e}^{-S_G(U)} \ , \ \beta \equiv rac{2N_c}{g^2}$$
 not the inverse temperature!

lattice spacing "a" disappeared"

# **Continuum limit**

long distance behavior of 2-point function:

$$egin{array}{lll} \langle \Gamma_n \Gamma_m 
angle &\sim {
m e}^{-M|n-m|} \ &\equiv {
m e}^{-|n-m|/{\pmb{\xi}}} \end{array}$$

 $\boldsymbol{\xi}$ : correlation length (statistical physics)

 $M \equiv \xi^{-1}$ : mass of a scalar particle in lattice units;  $M \equiv m_c a$ 

continuum limit: a 
ightarrow 0 , implies M 
ightarrow 0 for any fixed (physical) mass  $m_c$ 

$$M 
ightarrow 0 \ \Leftrightarrow \xi 
ightarrow \infty$$

 $\xi \rightarrow \infty$ : divergent correlation length  $\Rightarrow$ 

behavior of  $\pmb{\xi}$  defines the lattice spacing  $\pmb{\xi} \equiv c/a$ 

(2<sup>nd</sup> order) phase transition in statistical physics terminology



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### The continuum limit of lattice regularized QCD

- at present we consider only SU(Nc) gauge theories
- the only free parameter is the gauge coupling ~g~ or  $~eta=2N_c/g^2$

 $\Rightarrow g^2 \equiv g^2(a)$ 

Continuum limit:  $a 
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The gauge coupling  $g^2$  needs to approach a critical point  $g_*^2$  at which the 'correlation lengths', defined through 2-point functions, diverge, e.g.

$$G_2(ec{n})\equiv \langle \Gamma(0)\Gamma^\dagger(ec{n})
angle \sim {
m e}^{-ec{n}ec{n}ec{\xi}_{
m f}}$$

$$\hat{\xi}_{\Gamma} \equiv \hat{\xi}_{\Gamma}(eta) \equiv \hat{\xi}_{\Gamma}(g^2) = \xi_{\Gamma}/a$$

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$$G_{2}(\vec{n}) \equiv \langle \Gamma(0)\Gamma^{\dagger}(\vec{n}) \rangle \sim e^{-|\vec{n}|/\hat{\xi}_{\Gamma}}$$
$$\hat{\xi}_{\Gamma} \equiv \hat{\xi}_{\Gamma}(\beta) \equiv \hat{\xi}_{\Gamma}(g^{2}) = \xi_{\Gamma}/a \quad \stackrel{\text{<= often used notation}}{\underset{\text{but not quite correc}}{\overset{\text{= often used notation}}{\overset{\text{= often used notation}}{\overset$$

Continuum limit: physical observables,  $\Gamma = m_G, \ \sigma, \ r_1, \ \epsilon, \ \dots$  do not depend on the lattice spacing (cut-off)

$$a \frac{\mathrm{d}}{\mathrm{d}a} \Gamma = 0$$
 (1)

- observables calculated in a regularized QFT depend on the cut-off, e.g. they depend on the lattice spacing
- observables calculated on the lattice are dimensionless, i.e. they are calculated in appropriate units of the lattice spacing

$$\hat{\Gamma} \equiv a^{d_{\Gamma}} \Gamma$$

$$\hat{\Gamma} \equiv \hat{\Gamma}(g) \Leftrightarrow \Gamma = a^{-d_{\Gamma}} \hat{\Gamma} \equiv \Gamma(a,g)$$
(1) now reads:  $a \frac{d}{da} \Gamma = \left(a \frac{\partial}{\partial a} - \beta(g) \frac{\partial}{\partial g}\right) \Gamma = 0$ 
with  $\beta(g) = -a \frac{dg}{da}$   $\beta$ -function

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$$\hat{\Gamma} \equiv a^{d_{\Gamma}}\Gamma$$

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renormalization group equation
(1) now reads:  $a\frac{d}{da}\Gamma = \left(a\frac{\partial}{\partial a} - \beta(g)\frac{\partial}{\partial g}\right)\Gamma = 0$ 
with
$$\beta(g) = -a\frac{dg}{da}$$
 $\beta$ -function

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The  $\beta$ -function:  $\beta(g) = -a \frac{\mathrm{d}g}{\mathrm{d}a}$ 

$$\Leftrightarrow rac{1}{a} \mathrm{d}a = -rac{1}{eta(g)} \mathrm{d}g$$
 $\int_{a}^{a_0} rac{1}{a'} \mathrm{d}a' = -\int_{g}^{g_0} rac{1}{eta(g')} \mathrm{d}g'$ 

The  $\beta$ -function:  $\beta(g) = -a \frac{\mathrm{d}g}{\mathrm{d}a}$ 



The  $\beta$ -function

- controls the variation of the lattice spacing as function of the gauge coupling
- provides a solution to the renormalization group equation

The  $\beta$ -function:  $\beta(g) = -a \frac{\mathrm{d}g}{\mathrm{d}a}$ 

$$\Leftrightarrow \frac{1}{a} da = -\frac{1}{\beta(g)} dg$$

$$\int_{a}^{a_{0}} \frac{1}{a'} da' = -\int_{g}^{g_{0}} \frac{1}{\beta(g')} dg'$$

$$\ln(a_{0}/a) \Rightarrow \frac{a}{a_{0}} = e^{\int_{g}^{g_{0}} \frac{1}{\beta(g')} dg'} \equiv R(g, g_{0})$$
continuum limit:  $a \to 0 \quad \Leftrightarrow \quad \int_{g_{*}}^{g_{0}} dg' \dots \to -\infty$ 

$$\Leftrightarrow \quad \beta(g_*)=0$$

 $\beta$ -function needs to have a zero (fixpoint)

## **Asymptotic Freedom**

fixpoints:  $\beta(g_*) = 0$  $eta(q) = (q - q_*)^r \ b_0 \ , \ r \geq 1$ a special case:  $g_* = 0 \implies \frac{a}{r} = e^{\frac{1}{b_0(r-1)} \left(g^{-(r-1)} - g_0^{-(r-1)}\right)}$  $a\Lambda_L = \mathrm{e}^{-rac{1}{|b_0|(r-1)}rac{1}{g(r-1)}}$  $q 
ightarrow 0 \; \Leftrightarrow \; a 
ightarrow 0$ β**(g) QCD beta-function** r=3 ,  $b_0 < 0$  $eta(g) = -\left(rac{11N_c}{3} - rac{2n_f}{3}
ight)rac{g^3}{16\pi^2} + \mathcal{O}(g^5)$ **g**\* g b<sub>0</sub><0



M. Creutz, Phys. Rev. D21 (1980) 2308

Mike Creutz

F. Karsch, NNPSS 2017

## **Monte Carlo Simulations**

Observables = Expectation values

$$Z \;\;=\;\; \int {\cal D} {\cal A} {\cal D} \psi {\cal D} ar \psi \; {
m e}^{-S_E} \qquad \qquad \langle {\cal O} 
angle \;\;=\;\; {1\over Z} \int {\cal D} {\cal A} {\cal D} \psi {\cal D} ar \psi \; {\cal O} {
m e}^{-S_E}$$

integrate out fermions:

$$Z = \int \mathcal{D} \mathcal{A} \mathcal{D} \psi \mathcal{D} \bar{\psi} e^{-S_E} = \int \mathcal{D} \mathcal{A} \prod_f \det M(m_f) e^{-S_G} = \int \mathcal{D} \mathcal{A} e^{-S}$$
 $S = S_G - \sum_f \operatorname{Tr} \ln M(m_f)$ 

distribute gauge field configurations  $\{\mathcal{A}^{(i)}\}_{i=1}^{N_{tot}}$  according to the probability distribution  $P(\{\mathcal{A}\}) = Z^{-1}e^{-S(\{\mathcal{A}\})}$  Monte Carlo algorithms (detailed balance) generates Markov chain

calculate expectation values: 
$$\langle \mathcal{O} \rangle = \lim_{N_{tot} \to \infty} \frac{1}{N_{tot}} \sum_{i=1}^{N_{tot}} \mathcal{O}(\{\mathcal{A}^{(i)}\})$$

#### **Different regularization schemes** for fermions (and gauge sector)

 staggered fermions → doublers
 Wilson fermions → explict chiral symmetry breaking
 Domain Wall Fermions → 5-dimensional formulation, "almost" exact chiral symmetry, "residual mass"
 Overlap fermions → chiral fermion formulation (obeys Ginsparg-Wilson relation) chiral fermions are computationally demanding

overlap  $\sim 100 \, \mathrm{x}$  staggered

#### **Improved actions**

try to eliminate  $\mathcal{O}(a^2)$  discretization errors in the continuum limit

- pure gauge sector: Symanzik improvement, e.g. at 6-link terms to action - fermion sector: higher order discretization schemes, e.g. add three link terms: naïve staggered  $\rightarrow$  Naik action  $\rightarrow$  Highly improved staggered quarks (HISQ) Wilson fermions have  $\mathcal{O}(a)$  errors, add "clover-term" to arrive at  $\mathcal{O}(a^2)$